INVARIANT IMBEDDING AND MATHEMATICAL PHYSICS—I: PARTICLE PROCESSES

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SUMMARY

Using invariance principles in a systematic fashion, we shall derive not only new analytic formulations of the classical particle processes, those of transport theory, radiative transfer, random walk, multiple scattering, and diffusion theory, but, in addition, new computational algorithms which seem well fitted to the capabilities of digital computers. Whereas the usual methods reduce problems to the solution of systems of linear equations, we shall try to reduce problems to the iteration of nonlinear transformations.

Although we have analogous formulations of wave processes, we shall reserve for a second paper in this series a detailed and extensive treatment of this part of mathematical physics.

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Richard Bellman, Robert Kalaba and G. Milton Wing

Part I

INTRODUCTION

The classical equations of mathematical physics can be put in the form

$$(1) \qquad u_t = T(u)$$

where u is a vector function of a space vector p, restricted to a region R, and the time, $u = u(p,t)$. The operator T is in many cases a linear partial differential operator, in some cases a linear integral operator, and, if we insist upon realism, a nonlinear operator. The steady state version is obtained by setting the vector u_t equal to zero.

Since equations of this type usually have an infinite number of solutions, it is necessary to attach some further restrictions in order to single out a particular solution. To do this, we usually assign initial values,

$$(2) \qquad u(p,0) = v(p), \quad p \in R,$$

and boundary values

$$(3) \qquad u(p,t) = w(p,t),$$

for $p \in B$, the boundary of R.

Problems of this nature have two types of difficulties associated, difficulties which are, of course, inseparably intertwined, those of analytic character and those of computational nature. Among the many methods which have been proposed is the theory of semigroups. The guiding ideas were first enunciated by Hadamard, and subsequently were systematically pursued by Hille and Yosida; see Hille and Phillips, [1], for a thorough exposition and many references. Classically, the semigroup concept has been exploited in the time domain. Our aim is to show that this basic method can be applied in a much wider area, using other physical variables of significance as semigroup variables.

Using invariance principles in a systematic fashion, we shall derive not only new analytic formulations of the classical particle processes, those of transport theory, radiative transfer, random walk, multiple scattering, and diffusion theory, but, in addition, new computational algorithms which seem well fitted to the capabilities of digital computers. Whereas the usual methods reduce problems to the solution of systems of linear equations, we shall try to reduce problems to the iteration of nonlinear transformations.

Although we have analogous formulations of wave processes, briefly presented in [2,3,4], we shall reserve for a second paper in this series a detailed and extensive treatment of this part of mathematical physics.

Our interest in the field of invariance principles was aroused by the elegant and fundamental work of Chandrasekhar

in the theory of radiative transfer [30]. His results, in turn, are generalizations of those of Ambarzumian who seems to have been the first to have consciously employed invariance principles in any significant fashion [29]. Since then, in addition to our work, reference to which may be found at the end of the paper, there have been important contributions by Preisendorfer, [5,6], Ramakrishnan, [7], Redheffer, [8], and Ueno, [9,10,11]. In addition, there are some unpublished results due to Harris.

Independently, functional equation techniques were introduced into the theory of branching processes, in particular, those arising in cosmic ray cascade theory and biological mutation, by Bellman and Harris, [12,13], and Janossy, [14]. Surveys of the many results obtained over the last ten years may be found in Harris, [15,16], and Ramakrishnan, [17]. Also in the theory of dynamic programming, [18], in connection with the treatment of minimization and maximization problems, we find a use of invariance principles and functional equations which is quite similar in spirit to what we shall find below in the treatment of purely descriptive processes.

In place of beginning with an abstract formulation of particle processes and an abstract presentation of the principles of invariant imbedding, we shall start with a study of a particular process, neutron transport and multiplication. The difference in formulation between the usual approach and that furnished by "invariant imbedding," as we shall call our systematic application of invariance principles, will readily

be seen. Nevertheless, as we shall show, both are merely particular instances of a general approach.

Having gone through a spectrum of transport processes, steady-state and time-dependent, energy-independent and energy-dependent, one-dimensional and multidimensional, unchanging medium and Stefan-type, we shall abstract the basic ideas of invariant imbedding.

Following this, we shall apply these techniques to the study of random walk and multiple scattering, to the study of radiative transfer and diffusion. Our treatment of these fields will be much briefer since much of what is done in the part devoted to neutron transport can easily be transcribed and applied in these other areas.

In what follows, we shall pursue a purely formal path, leaving aside all questions of existence, uniqueness and so on. What is interesting, however, is that our approach enables us to handle many of these questions in a much simpler and straightforward way than that furnished by the conventional road.

Although we are in part motivated by a search for feasible computational techniques, we shall actually avoid any discussion of actual numerical techniques. In subsequent papers, we shall treat these matters in great detail. Here we shall restrain ourselves to generalities.

The equations of invariant imbedding are related to the variational formulas of Hadamard type, expressing the

dependence of the Green's function of a region upon the dimensions of the region (see [52]).

Finally, let us note that no previous knowledge of the equations of mathematical physics is required. All equations will be derived from first principles, directly from the mathematical model of the physical process.

Part II

NEUTRON TRANSPORT AND MULTIPLICATION

1. Introduction

Let us begin our journey with the examination of a number of intriguing mathematical problems which arise in the study of various aspects of neutron transport and multiplication. A consideration of some of the many different hypotheses that can be made will give us an opportunity to display the versatility of the theory of invariant imbedding.

Our basic assumption is that a neutron is a point particle which is completely specified at any time by its direction of motion and its energy. These two properties determine its state. As the neutron traverses the medium within which the transport process takes place, it suffers certain changes of state, i.e., changes in energy and direction, due to interactions with the medium and with other neutrons. In addition, we have the relatively new and very important phenomena of fission. Certain interactions can result in an increase in the number of neutrons, the fission process.

The probabilities of these events are measured by "cross-sections" or "mean free paths." Occasionally, we shall talk in deterministic terms, and occasionally in stochastic terms, depending upon which is more convenient. The difference is more apparent than real, since the use of expected values in a stochastic model leads to a completely deterministic version based upon fluxes.

Within the framework of a mathematical model constructed along these lines, a model we shall make more precise in the following section, we wish to explain and predict the phenomenon of criticality, and to determine the internal and external fluxes as functions of the spatial dimensions, the time and other parameters. Problems of this nature are of great complexity from the mathematical side, and thus of even greater fascination, even when greatly simplified physical models are used. When more realistic assumptions are made, the analytic aspects become truly formidable, and the problem of obtaining numerical results much more burdensome.

It is not to be expected that recondite scientific questions will yield readily to any single approach. Rather it is to be expected that with the aid of a battery of methods, each of which chips away at some of the obstacles in our path, we can eventually clear a road which will take us some distance toward our goal.

The classical equations of transport theory can be effectively applied in a number of cases. Approximate methods of various degrees of efficacy and associated results may be found in the book by Davison [19]. Rigorous discussion of these techniques can lead to quite complex analysis; see for example the papers by Lehner and Wing [20,21,44,49], Jörgens [43], and Pimbley [48].

A number of questions can be studied by means of the mathematical theory of branching processes. The study of age-independent processes was begun by Harris [15,16], and

Everett and Ulam, [22], independently of each other. Essentially it reduces to the study of the iteration of power series, with probabilistic overtones. The theory of age-dependent branching processes, based upon the systematic usage of functional equations, was begun by Bellman and Harris, [12,13], and independently by Janossy, [14]. Detailed expositions with many references will be found in the monograph by Harris, [15], and the expository papers by Harris, [16], and Ramakrishnan, [17].

It is natural to construct simplified models in a situation characterized by severe mathematical difficulties and by physical complexity as well. The usual hope is that the exploration of these models will furnish valuable experience and that the understanding of these more transparent models will enable us to penetrate into the more obscure versions. However, as mentioned above, even apparently simple processes give rise to sophisticated analysis.

Furthermore, as we shall discuss repeatedly below, unless the problems are carefully formulated they cannot be resolved in numerical terms in any straightforward fashion. Our objective in the pages that follow is to formulate a variety of transport processes in a way which will permit us to obtain numerical solutions with the aid of digital computers. As is often the case in mathematics and physics, a significant improvement in computational technique requires a new conceptual and analytic approach.

It turns out that in the process of fulfilling one of our goals, numerical solution of problems, we obtain as byproducts a host of interesting and elegant analytic results, together with powerful methods for establishing existence and uniqueness theorems for the associated functional equations and for the classical functional equations of mathematical physics. Many of these equations are quite difficult to treat along conventional lines.

Our principal tool will be the theory of invariant imbedding. Rather than attempt to define precisely what turns out to be more a state of mind than anything else, we shall first give a number of applications of the methods. Subsequently, we shall try to distill the essence of these.

2. A Simple Neutron Transport and Multiplication Process

Let us now describe a simple mathematical model of a neutron transport process with fission. Subsequently, we shall add a number of interesting features such as collision between neutrons, energy and time dependence, and so on. For the immediate purpose of illustrating both how the classical approach is made and how invariant imbedding techniques are used, there are great advantages to using the simplest possible version possessing certain structural properties.

As noted above, we take the neutron to be a point particle, and we allow at the moment only one-dimensional motion along a line, or part of a line. To simplify matters still further, we assume that there is no energy dependence. As this blithe,

carefree neutron moves along the line, it may suffer a collision with the constituent elements of the line. Again to simplify the algebra, we suppose that only fission collisions occur, resulting in one neutron moving to the left and one to the right. This is the only type of interaction we shall allow between the neutron and the transport medium at the moment. Furthermore, we shall suppose that there are no neutron-neutron interactions.

To make this verbiage precise, let us consider a finite interval $[0,x]$ (the reason for this apparently loose usage of x to designate an endpoint will be made clear subsequently. At the present, let us merely state that it is done with malice aforethought.), a one-dimensional rod, with the following properties:

(1) (a) When a neutron traverses an infinitesimal length Δ, in either direction, there is a probability $\sigma\Delta + o(\Delta)$* that fission will occur.

(b) When fission occurs, two neutrons are produced, one going to the right and one to the left. Each of these has the same properties as the original neutron.

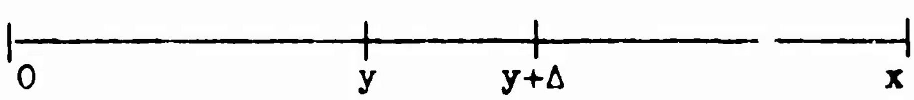

Fig. 1

*The notation $f(x) = o(g(x))$ is used to mean $\lim f(x)/g(x) = 0$, where the sense of the limit is usually obvious from the context.

(c) There is a probability $1 - \sigma\Delta + o(\Delta)$ that no interaction occurs in Δ, which means no change in the direction of the neutron.

(d) When a neutron leaves the rod, it cannot return and it has no further effect upon the transport process.

It would not be difficult to include absorption effects and collisions which merely change direction or to allow R neutrons, $R \neq 2$, out of a collision. Since these effects are treated subsequently, in multiple scattering, radiative transfer and random walk, we shall omit them here to keep the analytic details to an irreducible minimum.

The quantity σ is called the "macroscopic cross-section." Occasionally, we shall write it as $1/\lambda$, where λ is called the "mean free path." If the rod is homogeneous, these quantities are constant, otherwise we write $\sigma(y)$ and $\lambda(y)$ for the quantities associated with the interval $[y, y + \Delta]$.

We shall begin by considering steady-state neutron flux. The more general time-dependent case will be considered below. Let a unit flux of neutrons (that is, one neutron per unit time) be incident upon the right end of the rod, and let it be desired to determine the right and left fluxes at any internal point y, as well as the fluxes out at zero and x. These we shall regularly refer to as transmitted and reflected fluxes, respectively.

Our first formulation will be the classical one, resulting in simple versions of the linearized Boltzmann equation. Introduce the functions

(2) $\qquad u_R(y)$ = the expected number of neutrons going to the right at y per unit time,

$u_L(y)$ = the expected number of neutrons going to the left at y per unit time.

To obtain differential equations for u_R and u_L, we apply simple conservation laws for the right and left-hand flows at y. These are input-output equations expressing the fact that what goes out is the sum of what comes in and what is produced. By virtue of our assumptions concerning the transport and fission process and the elementary laws of probability, we obtain the equations

$$(3) \qquad \begin{aligned} u_R(y) &= u_R(y - \Delta)(1 - \sigma\Delta) + (u_R(y) + u_L(y))\sigma\Delta + o(\Delta), \\ u_L(y) &= u_L(y + \Delta)(1 - \sigma\Delta) + (u_R(y) + u_L(y))\sigma\Delta + o(\Delta). \end{aligned}$$

Passing to the limit as $\Delta \to 0$, we obtain the system of differential equations

$$(4) \qquad \begin{aligned} u_R'(y) &= \sigma u_L(y), \\ u_L'(y) &= -\sigma u_R(y). \end{aligned}$$

The boundary conditions are

$$(5) \qquad \begin{aligned} u_L(x) &= 1, \\ u_R(0) &= 0. \end{aligned}$$

These express the fact that there is an incident flux of unit strength at the point x, and the fact that there is no incident flux at the point 0. Observe a property which we shall repeatedly stress: The physical process automatically leads to a two-point boundary value problem when formulated in the foregoing way. The reason for discussing this fact will be discussed in detail below.

Finally, let us note that we can obtain the most general second order Sturm-Liouville equation from the foregoing process if we assume that right-hand motion at y has a different mean-free path than left-hand motion and that these mean free paths vary with y.

3. Invariant Imbedding Approach—Metaphysical

We now wish to formulate the transport process described in the foregoing section in different terms. Our approach will be based upon the theory of invariant imbedding. What we wish to do is to imbed the particular process considered above within a family of processes of similar nature. Although this appears to complicate rather than simplify the problem, its justification lies in the fact that there will exist simple relations between various members of the family which can be utilized to determine the characteristics of a particular member of the family.

The fact that the structure, or anatomy, of a particular organism can be understood quite readily in terms of the com-

parative anatomy of a phylum is well established in the field of biology. In chemistry, the construction of the Mendelieff-Moseley periodic table of the elements was a decisive step forward. In mathematics, the method of continuity is one of the basic devices of analysis and geometry. It follows that in pursuing this approach, we are invoking a factotum of science.

Consider the way in which an experimental physicist might study neutron flux in a rod. Starting with a rod of fixed length, he would measure reflected and transmitted fluxes. Increasing or decreasing the length, measurement would be made of the corresponding quantities. The final data would consist of two curves, one the reflected flux as a function of the length of the rod, the other the transmitted flux. These would be functions of x, the length of the rod.

Our aim here is to carry out the analytic equivalent of this program. In order for these concepts to be meaningful, we must find a way of relating the reflected and transmitted flux for a rod of length x with the corresponding fluxes for rods of different length. We propose then to consider the set of processes obtained by letting x assume any positive value. Our choice of the symbol x obviously presages this development.

One advantage of this approach as far as reduction of data is concerned is that it permits a direct comparison of analytic results with experimental results. The analytic and

computational advantages will be discussed in extenso below after we have supplied some analytic content to this metaphysical discourse.

4. Invariant Imbedding Approach—Analytical

We begin by introducing the function

(1) $u(x)$ = the expected number of neutrons reflected from $[0,x]$ per unit time as a result of an incident unit flux of neutrons per unit time at x.

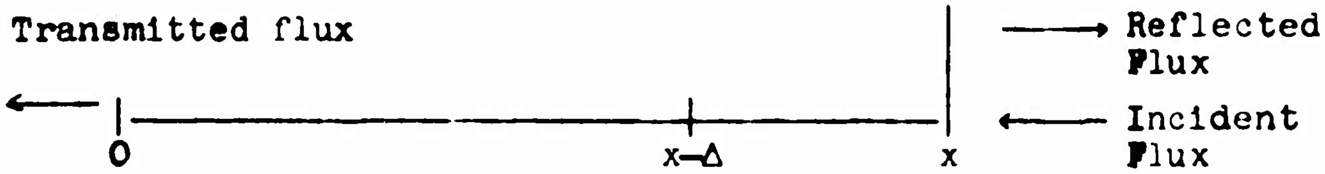

Fig. 2

Let us take Δ to be an infinitesimal. As the incident flux passes through the segment $[x - \Delta, x]$, some of the neutrons cause fission and others pass through unaffected to become incident upon $[0, x - \Delta]$. When a fission occurs in Δ one fission neutron emerges at x, while the other becomes a part of the incident flux at $x - \Delta$.

Some of the neutrons reflected from $[0, x - \Delta]$ may cause fission while passing through $[x - \Delta, x]$. The products of this fission yield a contribution to the reflected flux at x and furnish another source of neutrons incident upon $[0, x - \Delta]$.

Fortunately, although the physical process and mathematical counterpart are exceedingly complex if account of all fissions

and reflections is taken, this intricate bookkeeping is unnecessary if Δ is an infinitesimal. All other events, apart from those taken account of above, have a probability of occurrence of order Δ^2 or higher. Hence, they can be neglected in the derivation of the differential equation for the expected flux $u(x)$. Adding up the various effects and their associated probabilities, we obtain the equation

$$
\begin{aligned}
(2) \qquad u(x) &= \sigma\Delta(1 + u(x - \Delta)) \\
&\quad + (1 - \sigma\Delta)\left[u(x - \Delta)\left\{(1 - \sigma\Delta) + \sigma\Delta(1 + u(x - \Delta))\right\}\right] + o(\Delta).
\end{aligned}
$$

Letting $\Delta \longrightarrow 0$, we derive the differential equation

$$
(3) \qquad u'(x) = \sigma(1 + u^2(x)), \quad u(0) = 0.
$$

This first order nonlinear differential equation is called a Riccati equation. As we shall see, this type of quadratically nonlinear equation is characteristic of the equations derived by invariant imbedding techniques. In contrast, the classical equations are linear. Since we are describing the same process in different ways, there must be relations between the analytic descriptions. We shall obtain these below.

A further useful function is

(4) $\qquad v(x) =$ the expected transmitted flux per unit time as a result of a unit flux per unit time incident at x.

The same reasoning as above shows that $v(x)$ satisfies the equation

(5) $\quad v'(x) = \sigma u(x)v(x), \quad v(0) = 1.$

Observe that $u(x)$ satisfies a nonlinear differential equation whose solution is determined by an initial condition as compared to the linear equations for $u_R(y)$ and $u_L(y)$, determined by a two-point condition.

5. Connection Between the Two Approaches

It is clear that by suitable choice of y, we can obtain the functions $u(x)$ and $v(x)$ from the functions $u_R(y)$ and $u_L(y)$. Thus, if we make the dependence upon x explicit, we have

(1) $$u_R(y) = u_R(y;x),$$

$$u_L(y) = u_L(y;x),$$

and

(2) $$u(x) = u_R(x;x),$$

$$v(x) = u_L(0;x).$$

Can we, however, derive the internal fluxes $u_R(y)$ and $v_R(y)$, given the functions $u(x)$ and $v(x)$?

To accomplish this, we combine both viewpoints. Consider the following figure.

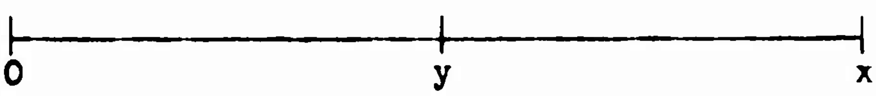

Fig. 3

To obtain a relation between $u_R(y)$, $u_L(y)$, and $u(y)$, we consider a source of strength $u_L(y)$ per unit time at y. Then the steady-state relation is clearly

$$(3) \qquad u_R(y) = u_L(y)u(y).$$

Similarly,

$$(4) \qquad u_L(y) = v(x - y) + u(x - y)u_R(y).$$

Hence, solving for $u_R(y)$ and $u_L(y)$, we have

$$(5) \qquad u_R(y) = \frac{u(y)v(x - y)}{1 - u(y)u(x - y)},$$

$$u_L(y) = \frac{v(x - y)}{1 - u(y)u(x - y)}.$$

It follows that we can consider $u(x)$ and $v(x)$ as fundamental functions from which all other functions can be derived.

6. Semigroup Properties*

Let us now obtain general relations connecting $u(x)$ and $v(x)$ with $u(y)$, $v(y)$ and $u(x - y)$, $v(x - y)$. The differential equations of §4 are particular cases of these relations.

Referring to the figure in §5 and tracing the multiply reflected and transmitted fluxes, we see that

*For a definition and discussion of semigroups see [1].

$$(1)\qquad u(x) = u(x - y) + v(x - y)u(y)v(x - y) + v(x - y)u(y)u(x - y)u(y)v(x - y) + \cdots = u(x - y) + \frac{v^2(x - y)u(y)}{1 - u(y)u(x - y)},$$

and similarly

$$(2)\qquad v(x) = \frac{v(x - y)v(y)}{1 - u(y)u(x - y)}.$$

Two values of particular interest are $y = \Delta$ and $y = x - \Delta$. The value $y = x - \Delta$ leads, as $\Delta \to 0$, to the foregoing differential equations, and the value $y = \Delta$ to Stokes' relations [51], a matter we shall discuss again below.

These results show that we can replace the solution of differential equations by the iteration of simple transformations. Consequently, these relations may be better suited for computational purposes than the foregoing differential equations.

7. A More General Imbedding

The foregoing results have essentially been consequences of the observation that the internal fluxes $u_R(y)$ and $u_L(y)$ are functions not only of y, the position at which they are measured, but also of x, the length of the rod. Hence, we should write, as already noted in §5,

$$(1)\qquad u_R(y) = u_R(y;x),$$

$$u_L(y) = u_L(y;x).$$

Consider now the more general situation in which we measure the fluxes at y due to a source at an internal point z.

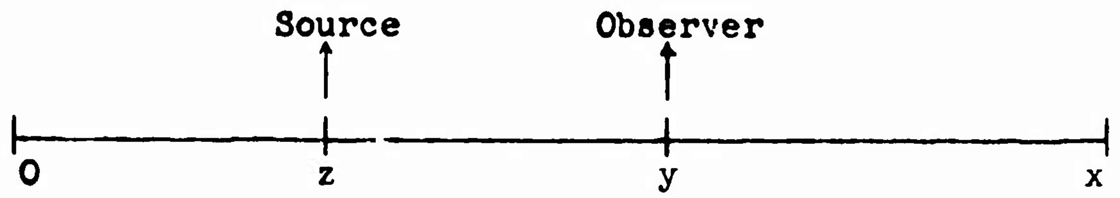

Fig. 4

The right-hand flux at y should now be denoted by $u_R(x,y,z)$ and the left-hand flux by $u_L(x,y,z)$. We are now at liberty to allow x, y and z to vary, either independently one at a time, or two at a time, or all three together.

We see then that there are at least three different ways in which we can imbed a particular process within a family of processes. Two of these, variation of y and z, lead to linear equations with two-point boundary conditions, while the third, variation with respect to x, leads to a nonlinear equation with an initial value condition. Each has certain analytic and computational advantages. In any particular situation, we employ the formulation which is most convenient. For further detail, see [23].

8. Energy Dependence (Multigroup Theory) [33]

Let us now turn our attention to a more realistic mathematical model in which we assume that a neutron is characterized by an energy level as well as a direction. In so doing, we have our choice of either a continuous range of energies, or a finite set of discrete levels.

In [23], we have discussed the continuous version. Let us concentrate upon the discrete version here, since this is a case of greater importance from the computational point of view. We shall begin, as before, with the conventional formulation.

The internal flux at y is now described by two vectors

(1) $$u(y) = \begin{pmatrix} u_1(y) \\ u_2(y) \\ \vdots \\ u_N(y) \end{pmatrix}, \quad v(y) = \begin{pmatrix} v_1(y) \\ v_2(y) \\ \vdots \\ v_N(y) \end{pmatrix}.$$

Here N is the number of distinct energy levels or groups, $u_i(y)$ represents the flux of neutrons in the i-th level to the right, and $v_i(y)$ the corresponding flux to the left.

Generalizing the foregoing model of a neutron transport process, we suppose that various interactions such as absorption, fission and non-fission collisions and so on, result in neutrons at one energy level being transformed into neutrons at other levels.

We introduce four matrices

(2) $$A = (a_{ij}), \quad B = (b_{ij}), \quad C = (c_{ij}), \quad D = (d_{ij})$$

where

(3) $a_{ij}\Delta$ = the expected <u>incremental</u> number of neutrons at the i-th level in the right-hand flux at $y + \Delta$, per neutron at the j-th level in the right-hand flux at y,

to within terms of order magnitude $o(\Delta)$. Similarly, $b_{ij}\Delta$ denotes the incremental contribution from left-hand to right-hand flux, $c_{ij}\Delta$ from right-hand flux to left-hand flux, and $d_{ij}\Delta$ from left-hand flux to left-hand flux. It should be noted that in the completely isotropic case the matrices A, B, C, D are closely related.

The usual conservation considerations lead to the equations

$$(4)\qquad \begin{aligned} u_i(y+\Delta) - u_i(y) &= \Delta \sum_{j=1}^{N} a_{ij}u_j(y) + \Delta \sum_{j=1}^{N} b_{ij}v_j(y) + o(\Delta), \\ v_i(y) - v_i(y+\Delta) &= \Delta \sum_{j=1}^{N} c_{ij}u_j(y) + \Delta \sum_{j=1}^{N} d_{ij}v_j(y) + o(\Delta), \end{aligned}$$

for $i = 1,2,\ldots,N$.

Letting $h \to 0$, we obtain the following vector-matrix equations:

$$(5)\qquad \begin{aligned} \frac{du}{dy} &= Au + Bv, \\ -\frac{dv}{dy} &= Cu + Dv, \end{aligned}$$

for $0 \leq y \leq x$.

As before, let us suppose that no neutrons are incident at 0, and there is a flux of intensity b_i per unit time of neutrons in the i-th level at x. We thus obtain the two-point boundary conditions

$$(6)\qquad u(0) = 0, \quad v(x) = b.$$

If the rod is inhomogeneous, the matrices A, B, C and D will depend upon y. Although there is no difference as far as the functional equation technique of invariant imbedding

is concerned between the treatment of the homogeneous and inhomogeneous, the classical treatment is simplified by the assumption of constancy of A, B, C and D. The discussion below applies equally to constant or variable matrices.

Let $W(y)$ be the matrix solution of

$$\frac{dW}{dy} = \begin{pmatrix} A & B \\ -C & -D \end{pmatrix} W, \quad W(0) = I. \tag{7}$$

To solve (5) subject to (6), we suppose that $v(0)$ has the as yet unknown value c. Then, the solution of (5) can be written

$$\begin{pmatrix} u(y) \\ v(y) \end{pmatrix} = W(y) \begin{pmatrix} 0 \\ c \end{pmatrix}. \tag{8}$$

Write

$$W(y) = \begin{pmatrix} W_{11}(y) & W_{12}(y) \\ W_{21}(y) & W_{22}(y) \end{pmatrix}, \tag{9}$$

where each W_{ij} is an $N \times N$ matrix. Using the terminal condition $v(x) = b$, we obtain the equation

$$W_{22}(x)c = b, \tag{10}$$

which determines the unknown vector c.

9. Computational Aspects

The determination of c in (8.10) requires the solution of a system of N linear equations in N unknowns. In

addition, we must determine the $N \times N$ matrix W using the linear differential equation in (7). Fortunately, since the equation is linear, we can determine $W(x)$ one column at a time. Hence, instead of the simultaneous determination of N^2 functions, we can perform N determinations of N functions.

10. Reflection and Transmission Matrices

Let us now consider the foregoing process using invariant imbedding techniques. To that end we introduce the matrix $R(x) = (r_{ij}(x))$, where

(1) $\quad r_{ij}(x) =$ the expected flux of neutrons in state i reflected per unit time from a rod of length x due to an incident flux at x of unit intensity per unit time in state j.

The same type of reasoning employed in the one-dimensional case yields the matrix equation

(2) $$R(x + \Delta) = B\Delta + (I + A\Delta)R(x)(I + D\Delta) + R(x)CR(x)\Delta + o(\Delta).$$

In the limit this yields the Riccati matrix equation

(3) $$R'(x) = B + AR + RD + RCR,$$

with the initial condition $R(0) = 0$.

In a similar fashion, if we introduce the transmission matrix $T(x) = (t_{ij}(x))$, where

(4) $t_{ij}(x)$ = the expected flux of neutrons in state i transmitted per unit time through a rod of length x due to an incident flux at x of unit intensity per unit time in state j.

Then, we obtain as before

(5) $T'(x) = T(D + CR)$.

11. Computational Aspects

The determination of $R(x)$, by way of (10.3), requires the simultaneous integration of N^2 nonlinear equations with the initial value $R(0) = 0$. This is a far more complicated operation than that of solving N sets of N linear equations, but, in recompense, it avoids the task of solving N simultaneous linear equations.

Furthermore, let us note that once $R(x)$ has been determined, we have resolved the transport process, determination of internal and external fluxes, for a set of rods of increasing length. On the other hand, the conventional method based upon linear equations yields the solution for one length at a time.

12. Criticality

Let us turn to a discussion of one of the most important phenomena associated with neutron transport and multiplication, namely criticality. As the length of the rod increases, the intensity of internal and emergent flux increases and becomes infinite as a certain critical length is attained.

To determine the critical length for the energy-independent case, let us begin with the linear equations of §2. Eliminating $u_L(y)$, we obtain the equation

$$(1) \qquad u_R''(y) = \sigma u_L'(y) = -\sigma^2 u_R(y).$$

We take σ constant for simplicity. The general solution is

$$(2) \qquad u_R(y) = c_1 \sin \sigma y + c_2 \cos \sigma y.$$

Using the two-point boundary conditions of (2.5), we readily obtain the equation

$$(3) \qquad u_R(y) = \sin \sigma y / \cos \sigma x.$$

We see then that $u_R(y)$ and $u_L(y)$ are infinite for $0 < y < x$ when $x = \pi/2\sigma$. This is the <u>critical length</u> for the simple neutron multiplication process we have set up.

Turning to the equation for the reflected flux obtained via invariant imbedding, we have

$$(4) \qquad u'(x) = \sigma(1 + u^2), \quad u(0) = 0,$$

whence

$$(5) \qquad u(x) = \tan \sigma x.$$

Once again, we see that $x = \pi/2\sigma$ is the critical length.

As pointed out by D. McGarvey, we can use (6.1) or (6.2) to obtain the critical length. In place of asking for the value of x which makes $u(x)$ infinite, it is sufficient to ask for the value of x which makes $u(x) = 1$, and then double x.

13. Criticality--Multigroup Case

It is in the determination of critical length in the energy-dependent case that the classical formulation encounters real trouble. To find the value of x which yields infinite flux, we must solve the determinantal equation

(1) $$\det (W_{22}(x)) = 0.$$

Let us note, once and for all, that when we speak of the critical value, we mean the smallest value of x which yields an infinite flux. From the physical point of view, the problem of determining expected fluxes is meaningless when the length of the rod exceeds the critical value. The higher values of x which yield infinite values are connected with the higher characteristic values associated with the two-point boundary-value problem. They do not appear to have any physical significance, although this is always a dangerous statement.

On the other hand, when we go over to a more sophisticated discussion concerning probabilities of fluxes of various intensity, and probability of fission, then it becomes quite significant to consider rods of greater than critical length. There are a number of interesting mathematical problems in this area which have been considered in detail by McGarvey, [24], and Mullikin and Snow, [25]. We shall discuss them briefly below.

Returning to the equation in (1), we see that if N, the number of groups, is of any size, say 10 or 20, the problem is not trifling. If $N = 50$ or 100, we cannot consider a solution along the foregoing lines to be satisfactory, for

a number of reasons which are familiar to numerical analysts.

The invariant imbedding technique requires the integration of N^2 simultaneous differential equations which are quadratically nonlinear. This integration is pursued until some element in the matrix $R(x)$ becomes infinite. To begin with, let us discuss the dimensional aspects. A computation of this type for $N = 10$ or 20 is completely routine for modern digital computers, and one of this nature for $N = 50$ is large, but feasible. For the machines that will be operational within a few years, values of N such as 100 or 200 will be routine.

Now let us turn to the integration of the differential equations until a singularity occurs. Clearly this is not a routine operation if accuracy is desired. There are several things that we can do. First of all, we can observe that as x approaches x_0, the critical value, we have an asymptotic behavior of the form

$$(2) \qquad r_{ij}(x) \sim \frac{s_{ij}}{(x - x_0)},$$

where $s_{ij} \geq 0$, and some $s_{ij} > 0$. Hence

$$(3) \qquad \frac{1}{r_{ij}(x)} \sim \frac{(x - x_0)}{s_{ij}},$$

when $s_{ij} > 0$. This linear behavior can be used to predict the value of x_0 with great accuracy. Furthermore, the fact that there are N^2 functions $r_{ij}(x)$ will enable us to determine x_0 with even greater accuracy.

Secondly, we can use McGarvey's observation, pointed out in the section on criticality for the simple energy-independent case. In place of finding the first value of x for which $R(x)$ is singular, we can ask for the first value of x for which the matrix $R(x)$ has its largest characteristic root equal to one. If this value is x_1, the critical value will be $2x_1$.

Since the matrix $R(x)$ is a positive matrix, or at least, nonnegative, we know that there will be one root of largest absolute value which is real [53]. By slight perturbation of the transition matrices A, B, C, and D we can actually ensure that all the entries in $R(x)$ are positive, which means that the root with largest absolute value will actually be positive.

There are now available a number of simple and efficient techniques for determining this root, the Perron root, of a positive matrix. Furthermore, since clearly $R(x)$ has monotonically increasing elements, we can use various interpolation methods to locate the position of this root very accurately. A large number of questions in the theory of branching processes can be reduced to the problem of determining the largest characteristic roots of positive operators; see Bellman-Harris, [26], Birkhoff, [27].

In any case, this method seems far superior to that of finding the roots of a determinantal equation of high degree. It would seem that invariant imbedding techniques have a distinct advantage as far as the determination of critical parameters is concerned.

14. Extrapolation over Multigroups

One way of determining the critical length with great accuracy is based upon the use of a large number of energy levels. It is reasonable to suspect that closer and closer values to the true value will be derived as we use finer and finer subdivisions of the energy range. Consequently, we can use the following extrapolation method. Solve the problem for $N = 10$, for $N = 20$, $N = 30$, and so on, until we reach the limits of the computer. Using the successive values obtained for the critical length, we can extrapolate to $N = \infty$, and thereby obtain a more precise value.

Here is where an analysis of the precise asymptotic form as $N \rightarrow \infty$ will be very valuable. With the aid of an analytic representation of the critical length as a function of N, we can use superior extrapolation procedures.

Of course, it is seldom possible to obtain cross sections and other physical parameters, as continuous functions. Hence the limiting case, $N \rightarrow \infty$, is often of greater mathematical interest than it is of physical importance.

15. Multidimensional Transport Theory--Slab Case

Leaving the physically cramped but mathematically comfortable confines of the one-dimensional, let us begin our investigation of the more significant multidimensional processes by considering a neutron transport process taking place in an infinite slab contained between the planes $y = 0$ and $y = x$ in three space. As usual, surrounding the slab is a

vacuum which means that a neutron leaving the slab at either boundary never returns.

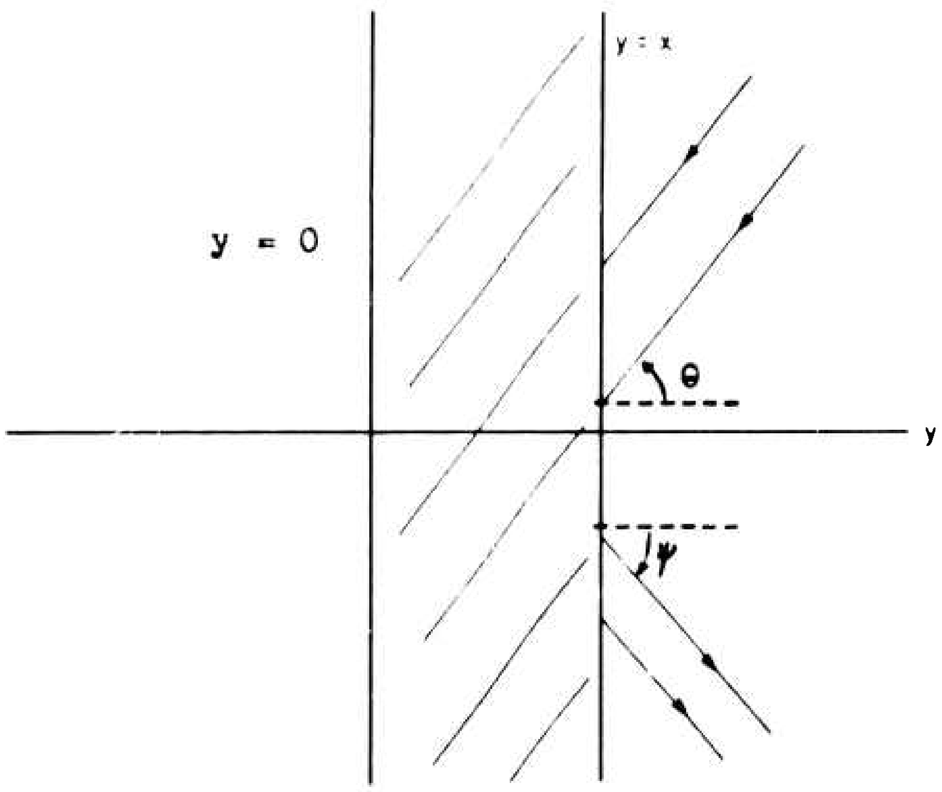

Fig. 5

A classical formulation of this problem leads in the isotropic case to the equation

$$(1) \qquad \frac{1}{c}\frac{\partial f}{\partial t} + \mu \frac{\partial f}{\partial y} + \sigma f = \frac{k\sigma}{2}\int_{-1}^{1} f(x,\mu',t)\,d\mu',$$

where c is the constant neutron velocity, σ is the constant collision cross-section and k is the average number of neutrons emerging from a collision. As usual, μ is the

cosine of the angle between the direction of motion of the particle and the positive y-direction, and $f(y,\mu,t)$ is the density of neutrons at y traveling in direction μ at time t.

There are boundary conditions at $y = 0$ and $y = x$, arising from the fact that particles may not reenter the slab once they have emerged. In the steady-state situation, of the type we have so far been considering, (1) takes the form

$$(2) \qquad \mu \frac{\partial f}{\partial y} + \sigma f = \frac{k\sigma}{2} \int_{-1}^{1} f(x,\mu',t)d\mu' .$$

A rigorous treatment of Equations (1) and (2) requires deep analysis; see [20,21].

Let us consider this problem using invariant imbedding techniques. To simplify our initial presentation, let us return to neutrons which are independent of energy, but do, however, possess directions of motion. Assume, as indicated in the picture above that there is a plane parallel flux in direction θ per unit area per unit time incident at x, and that we are given the various probabilities of absorption, scattering and fission collisions, and the resultant angular distribution of neutrons.

The type of reasoning used in the previous sections enables us to derive a functional equation of the form

$$(3) \qquad \frac{\partial u}{\partial x} = T(u),$$

where T is a quadratic operation, for the function

(4) $u(x,\theta,\psi)$ = the reflected flux per unit area on the surface in the ψ-direction per unit time as a result of a unit incident flux per unit area on the surface per unit time.*

There is no need for us to go into the details for three reasons. In the first place, we shall derive similar equations below for cylindrical and spherical geometries. The second reason we shall discuss immediately below. Finally, we shall discuss this problem from another physical viewpoint in Part V.

16. Equivalence of One-dimensional Energy-dependent Case and Angular-dependent, Energy-independent Slab Case

What is important is the observation that the transport process for a one-dimensional rod with energy-dependence is abstractly equivalent to the process for the slab with discrete angular dependence, but no energy dependence.

In both cases, we have a finite number of "states" and mechanisms for transforming a neutron from one state to another. Another advantage of this formulation lies in the fact that the inclusion of energy dependence in the slab merely increases the number of states, without at all changing the mathematical formulation.

17. Cylindrical Regions

The infinite slab is stratified by considering it to be composed of a series of strata of which the stratum between $y = x$ and $y = x - \Delta$ is typical (Figure 6).

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*Throughout this paper we measure fluxes with respect to the geometrical areas on which they impinge, rather than with respect to a plane normal to the beam. For a discussion, see §59.

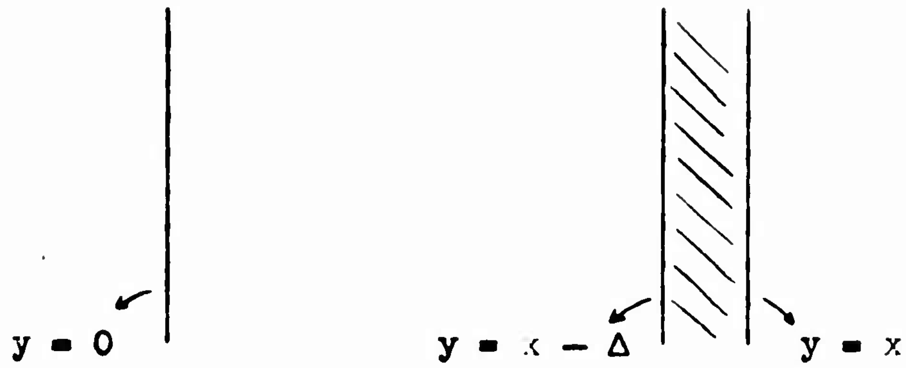
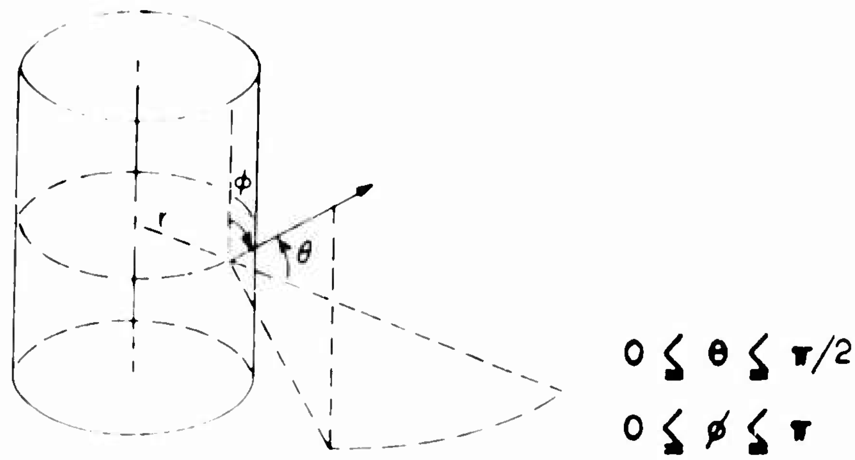


Fig. 6

In analogous fashion, we can stratify other regions with various types of symmetries. Consider, for our first example of this, an infinite cylindrical region, whose cross-section $\sigma(r)$ is dependent only upon the radial coordinate r. Let us suppose that neutron production is energy independent and isotropic, with k neutrons emerging after each collision.

Given an incident flux of one neutron per unit area per unit time on the surface at angles (θ,ϕ), we wish to determine the reflected flux $\Psi(r,\mu,\phi,\mu',\phi')$. As usual, $\mu = \cos\theta$ (Figure 7).

The imbedding is now performed by considering the cylindrical region to be composed of a sequence of infinitesimal cylindrical shells. In cross-section, they appear as in Figure 8.



(For ingoing particles, θ is measured with respect to the inward normal.)

Fig. 7

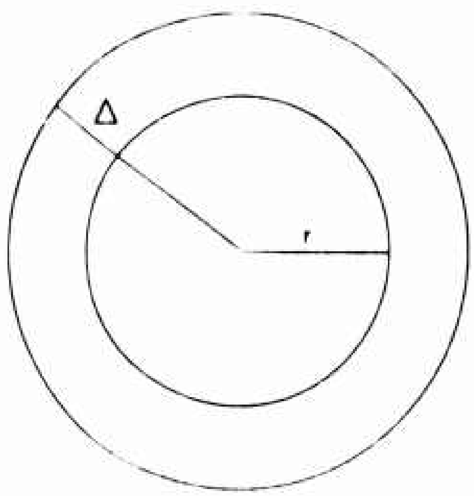


Fig. 8

Referring to the foregoing two figures, and adding up effects as before, we obtain the functional equation (see [47])

$$(1)\quad \frac{d\psi}{dr} = \frac{q\sigma(r)\csc\phi}{4\pi\mu} + \frac{q\sigma(r)\csc\phi}{4\pi\mu}\int_0^{\pi} d\phi'' \int_0^{1} \psi(r,\mu'',\phi'',\mu',\phi')\,d\mu''$$

$$- \frac{\sigma(r)}{4\pi}\left[\frac{\csc\phi}{\mu} \quad \frac{\csc\phi'}{\mu'}\right]\psi(r,\mu,\phi,\mu',\phi')$$

$$+ \frac{g\sigma(r)}{4\pi} \int_0^{\pi} d\phi'' \int_0^1 d\mu'' \psi(r,\mu,\phi,\mu'',\phi'') \frac{\csc\phi''}{\mu'}$$

$$\cdot \left\{ 1 + \int_0^{\pi} d\phi''' \int_0^1 d\mu''' \psi(r,\mu''',\phi''',\mu',\phi') \right\},$$

$$\psi(0,\mu,\phi,\mu',\phi') = 0.$$

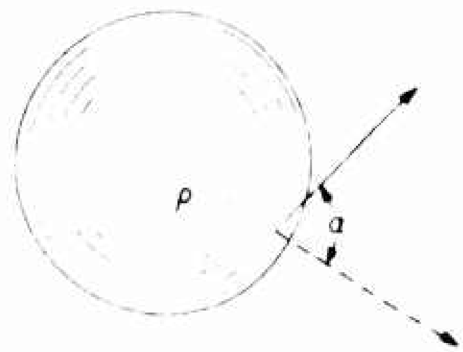
To compute $d\psi/dr$ we must note that μ itself is really a function of r, and the same is true of μ'. Upon taking this into consideration we find

$$(2) \qquad \frac{d\psi}{dr} = \frac{\partial\psi}{\partial r} + \frac{\partial\psi}{\partial\mu} \frac{1-\mu^2}{\mu r} + \frac{\partial\psi}{\partial\mu'} \frac{1-\mu'^2}{\mu' r}.$$

We shall discuss the corresponding result for spherical regions, and then discuss the computational significance of these results.

18. Spherical Regions

As our next example, consider a sphere composed of transport material whose cross-section is dependent upon the radial coordinate ρ alone. As indicated in the following figure, we introduce an angular coordinate α, $\cos\alpha = v$, and suppose that we have a conical flux of neutrons, with direction v, incident uniformly over the surface of the sphere, one neutron per unit area per unit time. We wish to determine the reflected flux in direction v', $\psi(\rho,v,v')$.



$0 \leq \alpha \leq \pi/2$

Fig. 9

The usual analysis yields the equation [47]

$$(1) \quad \frac{\partial \Psi}{\partial \rho} + \frac{1 - v^2}{v\rho} \frac{\partial \Psi}{\partial v} + \frac{1 - v'^2}{v'\rho} \frac{\partial \Psi}{\partial v'}$$

$$= \frac{q\sigma(\rho)}{4\pi v} + \frac{q\sigma(\rho)}{2v} \int_0^1 \Psi(\rho, v'', v')dv''$$

$$- \sigma(\rho)\left(\frac{1}{v} + \frac{1}{v'}\right)\Psi(\rho, v, v')$$

$$+ \frac{q}{2}\sigma(\rho) \int_0^1 dv'' \frac{\Psi(\rho, v, v'')}{v''} \left\{1 + 2\pi \int_0^1 \Psi(\rho, v''', v')dv'''\right\}.$$

19. Critical Mass

The critical reader may seriously question the value of the results obtained in the two previous sections, since incident fluxes of the type we have employed are seldom found. This is certainly a valid criticism.

There is, however, one quite important case in which we can profitably use this type of flux, and, indeed, whatever type of flux is most convenient. This is the determination of critical mass. It is possible to convince oneself that whatever

radius is critical for one type of flux will be critical for any other type of steady-state flux.

20. More General Fluxes

The same persevering reader may also ask why we have not used invariance principles directly for more general fluxes. This can be done. What has held us back has been dimensionality difficulties. Consider, for example, a two-dimensional slab in which we consider an incident flux of unit intensity per unit time at an angle θ at a particular point, say $z = 0$.

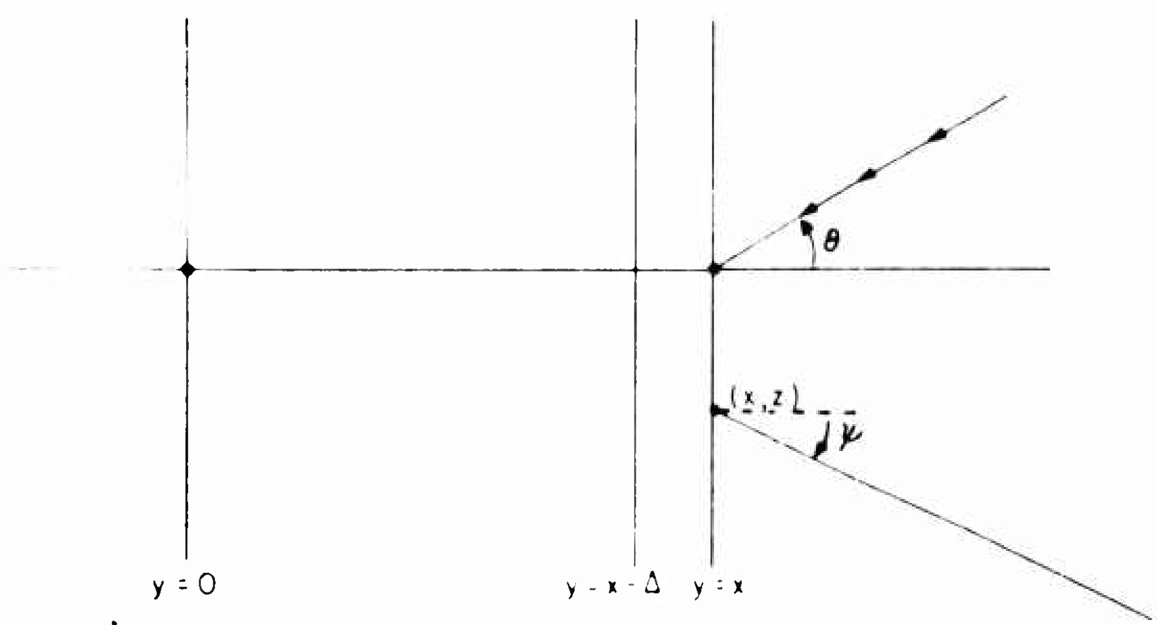


Fig. 10

We then introduce the flux, $u(\theta,\psi,z,x)$, as the reflected flux at angle ψ per unit time at the point a distance z

from the point of incidence. We then obtain the same type of equation for u as before, with the difference that u now depends upon one additional variable z. This increase in dimensionality introduces formidable computational difficulties due to the enormously increased memory requirements.

From the analytic point of view, there is no difficulty in considering realistic fluxes. From the computational point of view, these more realistic problems require new techniques and bigger and faster machines. For a possible line of approach, see [28].

21. Volterra versus Fredholm Equations

The equations we have obtained in the foregoing sections using invariant imbedding techniques have invariably been nonlinear, as compared to the linear equations of classical transport theory. Considering the fact that linear equations with their superlative superposition properties are difficult enough to analyze theoretically and resolve numerically, why do we wish to introduce nonlinear equations? Although we have gnawed around the edges of this question in previous pages, let us now make it the principal course.

Our answer can be put in very simple terms: We wish uniformly to replace two-point boundary value problems, and boundary-value problems in general, by initial value problems. This is equivalent to replacing Fredholm-type integral equations by Volterra-type integral equations. Naturally, the equations will be in different variables.

This is not a new idea, and, indeed, is one that has been proposed before, and used with some success. The approach we use, however, based upon invariance principles, and extending that of Ambarzumian, [29], and Chandrasekhar, [30], is quite different from these mentioned, and quite unlike any earlier methods.

We are engaged in this program for two reasons. In the first place, Volterra-type equations lead to iterative algorithms which are simpler for digital computers than algorithms based upon the solution of linear systems of equations. Secondly, and the two are intimately related, functional equations of the type we derive, despite their nonlinearity, are easier to treat as far as existence and uniqueness are concerned. These last topics, however, we have bypassed here since we are at the moment principally interested in exhibiting the mechanics of the formulation of the classical particle processes in these new terms.

22. Stokes Relations

It is interesting to find that the reflection and transmission matrices, and, more generally, the reflection and transmission functions, are related to each other in algebraic fashion. We already have the Riccati differential equation for $R(x)$ and the differential equation for $T(x)$ in which $R(x)$ enters (see §10).

We shall refer to these new relations as Stokes'

relations since the first identities of this type connecting reflection and transmission coefficients were discovered by Stokes in work on light rays impinging on slabs.

In § 6, we discussed the semigroup properties of the functions $u(x)$ and $v(x)$ obtained for the simple one-dimensional energy-independent process. Recognition of these transformation properties is also found in Redheffer, [31]. and for the matrix case as well. To obtain the following relations, we use the special case of these relations in which the stratification instead of being as before,

Fig. 11

is, instead,

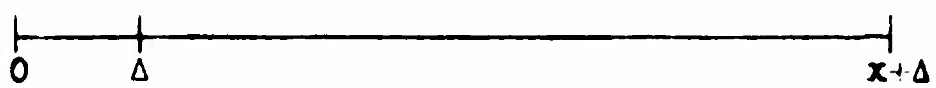


Fig. 12

where Δ is an infinitesimal.

The usual counting process yields the relation

$$R(x + \Delta) = R(x) + T(x)BT(x)\Delta + o(\Delta), \tag{1}$$

or

$$(2) \qquad R'(x) = TBT.$$

In view of Equation (10.3), we conclude that

$$(3) \qquad TBT = B + AR + RD + RCR,$$

a relation which is not too easy to verify directly.

Similarly, we find that

$$(4) \qquad T(x + \Delta) = (I + D\Delta)T(x) + R(x)BT(x)\Delta + o(\Delta),$$

whence

$$(5) \qquad T'(x) = (D + RB)T.$$

This in conjunction with Equation (10.5) yields the further result

$$(6) \qquad T(D + CR) = (D + RB)T.$$

23. Probabilities

For various purposes, it is desirable to have a more precise picture of the transmitted and reflected flux than that furnished by the expected values. This is particularly the case when x is just less than critical, when it assumes the critical value, and when x is greater than critical, the case of supercriticality.

Let us then talk about the probabilities of events, rather than the expected events. In place of a steady-state situation, let us suppose that one neutron is incident at x,

the right end of our one-dimensional rod, at time zero. We shall call this neutron the <u>trigger neutron</u>.

Let us define the set of probabilities

(1) $p_n(x)$ = the probability that n neutrons are reflected from a rod of length x over all time as a result of one trigger neutron incident at x at time zero.

In order to obtain a set of differential equations for these functions, we observe that the trigger neutron incident upon a rod of length $x + \Delta$ either has a fission collision in the initial length $[x + \Delta, x]$ or it does not. If it does not, consider the neutrons that emerge from the length $[0, x]$. If k of these emerge over all time, then at most one of these, to terms in $o(\Delta)$, can have a fission collision in the interval $[x, x + \Delta]$. Consideration of these possibilities, together with that of an initial fission collision, leads to the relation

(2) $$p_n(x + \Delta) = (1 - \sigma\Delta)\left\{p_n(x)(1 - n\sigma\Delta) + \sum_{k=1}^{n} p_k(x) k\sigma\Delta p_{n-k}(x)\right\}$$

$$+ \sigma\Delta p_{n-1}(x) + o(\Delta),$$

$$n = 0, 1, 2, \ldots; \quad p_{-1}(x) = 0.$$

Passage to the limit yields the infinite system of differential equations

$$(3) \qquad p_n'(x) = -(n+1)\sigma p_n(x) + \sigma p_{n-1} + \sigma \sum_{k=1}^{n} k p_k(x) p_{n-k}(x),$$

$$n = 0,1,2,\ldots; \quad p_{-1}(x) = 0.$$

Physical considerations yield the obvious boundary conditions

$$(4) \qquad p_n(0) = \begin{cases} 1, & n = 0 \\ 0, & n \neq 0. \end{cases}$$

In order to test the feasibility of the computational solution of systems of this type, and to obtain some idea of the time required, the first forty of these equations were solved numerically using a rather old-fashioned machine, the RAND Johnniac. Graphs of the results may be found in [32] and [33].

A number of interesting questions concerning the analytic behavior of the $p_n(x)$ as x approaches the critical value arise as a result of these computations.

If we introduce the generating function

$$(5) \qquad u(x,s) = \sum_{n=0}^{\infty} p_n(x) s^n,$$

we readily obtain the quasilinear partial differential equation

$$(6) \qquad u_x = \sigma(s-1)u + \sigma s(u-1)u_s,$$

with the initial condition

$$(7) \qquad u(0,s) = 1.$$

This equation has been studied in detail by Mullikin and Snow, [25]. The solution exhibits a very strange behavior as x goes through the critical value. As we shall see below, the equation for the generating function can be obtained immediately by means of functional equation techniques.

It is important to insert a word of caution about the use of these techniques. Methods based upon expected values can be used with a carefree abandon as long as the length of the rod is less than critical. On the other hand, the probabilistic equations obtained above hold for any value of the rod. They must be considered the basic equations.

As long as x is less than the critical length, we have the condition

$$(8) \qquad \sum_{n=0}^{\infty} p_n(x) = 1$$

in addition to the initial values of (4). As soon as x is greater than the critical length, this equation no longer holds. This is due to the fact that there is now a new probability to be added, the probability of an infinite flux. Lack of recognition of this fact can lead to paradoxical conclusions. A thorough discussion of this phenomenon will be found in the paper by Mullikin and Snow cited above.

Finally, let us note that similar equations can be obtained for the transmission probabilities, see [32].

24. Analogy between Critical Length and Initiation of Shock Wave

The equation for the generating function, given above in §23, is analogous to the equation

$$u_t = uu_x, \tag{1}$$

where t is now a time variable and ace variable, used by Courant—Hilbert, and others, as xample of how a discontinuity can arise in the behavior of the solution of a differential equation. This type of discontinuity is similar to that which is observed in the behavior of blast waves and is called a "shock."

It is interesting then to observe this analogy between the onset of a shock as a function of time and the onset of criticality as the length, or radius, is increased. Analogies of this type are useful since knowledge gained in one area can then be easily transplanted to another.

We shall observe a further analogy subsequently. Just as the presence of the smallest degree of viscosity destroys the pure shock, so the presence of the slightest neutron—neutron interaction can destroy criticality (see [34]).

25. Description of a Generalized Transport Process

As we shall see in a moment, the imbedding technique, which we have used so far only for one—dimensional rods, slabs, cylindrical and spherical regions, can be considerably extended. Let us now formulate a transport process in general terms. Let a family of surfaces in

n-dimensional space be characterized by a single continuous parameter $\eta \geq 0$. The surface corresponding to $\eta = 0$ (it may be a degenerate surface) will be considered a bounding surface, and the parametrization will be such that the region included between $\eta = 0$ and $\eta = \eta_1$ will be included by the region between $\eta = 0$ and $\eta = \eta_2 > \eta_1$. It is clearly not necessary to consider the topological properties of these surfaces and regions in detail. Such ideas as outward and inward directions, area of a surface, and so on, can be taken intuitively as far as our purposes are concerned. The family of surfaces will be assumed to partition continuously all or part of the n-dimensional space into a set of strata.

For example, the family of surfaces may be the set of all spheres centered at the origin in three-dimensional space. Here η is r, the radius of the sphere, and $\eta = 0$ is a degenerate bounding surface, a point sphere. Again, the family may be the set of all vertical lines, in the two-dimensional space, to the right of the vertical axis. In this case we can choose η to be x, and $x = 0$ is a nondegenerate bounding surface.

By a "particle" we shall understand a state vector S depending on the parameter η. The state vector contains information regarding the direction of motion, energy, specific location on η, the type or types of physical particles that we are discussing (in case there are particles other than neutrons), and any other properties which we may choose to include in the process.

The stratum $(\eta, \eta + \Delta)$, $\Delta > 0$, will be assumed to contain a medium which permits a transport process. A particle passing through the stratum may engage in interactions of both a deterministic and a stochastic nature. As mentioned above, the distinction between these is really a matter of mathematical convenience. The deterministic interactions will produce effects which will be proportional in magnitude to Δ plus a term $o(\Delta)$; the stochastic interactions will have <u>probability</u> of occurrence proportional to Δ plus $o(\Delta)$ within the stratum $(\eta, \eta + \Delta)$. These interactions will have no effect on the transport medium, but will result in a transformation on the state vector S, in some cases transforming it into two or more such vectors (fission), in some cases annihilating it (absorption), in other cases leaving one vector as before. Hence, the movement of a particle within the medium between 0 and η can be thought of as a sequence of transformations on state vectors, together with the creation and annihilation of vectors. Subsequently, in §36, we shall consider a process in which the medium is changing as the process continues.

We shall now investigate the following problem. Let a flux of "particles" specified by S impinge on η. What are the number and nature of the particles (state vectors) emergent from η? Often the source will be given in particles per unit time, in which case we shall seek the number of particles emerging from η per unit time. In some

instances, we shall be concerned with the number and nature of particles emergent from $\eta = 0$ per unit time? The former particles we shall call "reflected," the latter we call "transmitted." It is clear that in some cases, such as for the sphere mentioned above, the second problem is ill-posed. We shall investigate only the problem of reflection, since the formulas for transmission can be obtained in a similar fashion.

26. The Expected Value Equation

We begin by considering not the state vector itself, but its expected value. Consider a stream of particles, one per unit area per unit time, in state S, impinging upon the surface η. We ask for the expected number, or flux, of particles in state S' reflected per unit area per unit time. Denote this flux by $\Psi(\eta,S,S')$. For the present discussion we shall assume that S and S' contain no information about the specific location on η. It is evident that this assumption imposes a strong symmetry requirement upon both the surface η and the impinging flux.

Let the probability that a particle in state S passing through $(\eta,\eta \pm \Delta)$ suffers a collision—the stochastic process—be given by $P(\eta,S)\Delta + o(\Delta)$. Let $T(\eta,S,S')$ be the average number of particles in state S' resulting from this interaction and transmitted to $\eta \pm \Delta$. Let $R(\eta,S,S')$ be the average number in state S' reflected back to η. Then, proceeding as above, we find

$$
\begin{aligned}
(1)\quad \Psi(\eta+\Delta,S,S') = {} & P(\eta,S)\Delta R(\eta,S,S') \\
& + P(\eta,S)\Delta \int_{S''} T(\eta,S,S'')\Psi(\eta,S'',S')dS'' \\
& + [1 - P(\eta,S)\Delta]\Psi(\eta,S,S')[1 - P(\eta,S')\Delta] \\
& + [1 - P(\eta,S)\Delta] \int_{S''} dS''\Psi(\eta,S,S'')\Delta P(\eta,S'') \\
& \cdot \left\{T(\eta,S'',S') + \int_{S''} R(\eta,S'',S''')\Psi(\eta,S''',S')dS'''\right\} \\
& + o(\Delta).
\end{aligned}
$$

The first term on the right-hand side of this equation represents the contribution to the reflected flux from the particles which are reflected immediately from the stratum of thickness Δ, and the second arises from those which pass through this stratum but change state, giving reflected particles from $[0,\eta]$ which then pass through the stratum without interaction. The third term is produced by particles which pass unaffected through $[\eta,\eta+\Delta]$ and give rise to reflected particles from $[0,\eta]$ which again pass through the stratum without interaction. The last term accounts for particles which enter $[0,\eta]$ without interaction in $[\eta,\eta+\Delta]$, but whose reflected flux does have an interaction in $[\eta,\eta+\Delta]$. Some of this flux is transmitted through this stratum, the rest is returned to $[0,\eta]$ and re-reflected.

Here all the states on the right-hand side are taken at η, and the integration over states is symbolic. The transport equation resulting when $\Delta \to 0$ is then

$$(2) \quad \frac{\partial\Psi}{\partial\eta} = P(\eta,S)R(\eta,S,S') + P(\eta,S)\int_{S''} dS''T(\eta,S,S'')\Psi(\eta,S'',S')$$

$$- \left[P(\eta,S) + P(\eta,S')\right]\Psi(\eta,S,S')$$

$$+\int_{S''} dS''\Psi(\eta,S,S'')P(\eta,S'')\Big\{T(\eta,S'',S')$$

$$+\int_{S'''} dS'''R(\eta,S'',S''')\Psi(\eta,S''',S')\Big\}.$$

It may be shown that (2) includes Equations (17.1) and (18.1) as special cases. By choosing different geometries and different meanings for S it is possible to write down a great variety of particular transport equations using this general result. For more details, see [4].

27. A Simple Stochastic Case

Before attempting to write down a general stochastic functional equation, we consider a simple example, the first of §2. We assume, for further simplicity, that in a collision exactly two neutrons emerge, one going to the right, one to the left. We let one neutron enter the bar at time zero.

Let $\left\{U^{(i)}(x)\right\}$, $i = 1,2,3,\ldots,$ be a sequence of random variables denoting the number of neutrons reflected from the bar in all time. Let $\left\{F^{(i)}(\Delta)\right\}$, $i = 1,2,3,\ldots,$ be another sequence of random variables with

$$F^{(i)}(\Delta) = \begin{cases} 1 & \text{if a collision occurs in a segment of length } \Delta, \\ 0 & \text{otherwise.} \end{cases}$$

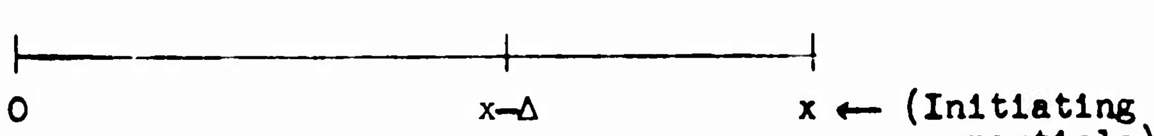


Fig. 13

Then, using the invariant imbedding principle, we have

$$(1)\quad U^{(1)}(x) = F^{(1)}(\Delta)\left\{1 + U^{(2)}(x-\Delta)\right\} + (1 - F^{(1)}(\Delta)) \sum_{i=4}^{U^{(3)}(x-\Delta)+4} \left\{1 + F^{(1)}(\Delta)U^{(1)}(x-\Delta)\right\} + w(x,\Delta),$$

where $\text{Prob}\left\{w(x,\Delta) \neq 0\right\} = o(\Delta)$.

Let us interpret this equation. The superscripts in themselves have no significance and serve merely to distinguish one random variable from another. Notice that if the initiating particle makes a collision in passing from x to $x - \Delta$ (Fig. 13), the second term of (1) is zero while the first gives just the number of particles emergent from $x - \Delta$ —namely, the one immediately out due to the collision in $(x - \Delta, x)$ plus the random number $U^{(2)}$ due to the left moving neutron acting as a source particle for the rod $(0, x - \Delta)$. If there is no initial interaction in the interval $(x - \Delta, x)$, then the first term of (1) is zero, and the second term counts. Of the random number $U^{(3)}(x - \Delta)$ of neutrons emerging from $x - \Delta$ some make no collisions in $(x - \Delta, x)$ and hence contribute only one to the sum. Others make a collision in $(x - \Delta, x)$ giving not only an immediate right traveling particle, but also a random number $U^{(1)}(x - \Delta)$ reflected from $(0, x - \Delta)$. The fact that all other processes are "unlikely" is included in the term w.

We now introduce the generating function

(2) $$u(x,s) = E\{s^{U(x)}\}.$$

Then, using the properties of the generating function and writing $\text{Prob}\{F^{(1)}(\Delta) = 1\} = \sigma\Delta + o(\Delta)$, we find, after careful calculation with (1), the equation

(3) $$\begin{aligned} u(x,s) &= \sigma\Delta s u(x - \Delta,s) \\ &\quad + (1 - \sigma\Delta)u(x - \Delta,(1 - \sigma\Delta)s + \sigma\Delta s u(x - \Delta,s)) + o(\Delta) \\ &= \sigma\Delta s u(x,s) + (1 - \sigma\Delta)[u(x - \Delta,s) \\ &\qquad + u_s(x - \Delta,s)(- \sigma\Delta s + \sigma\Delta s u)] + o(\Delta). \end{aligned}$$

This leads at once to the partial differential equation

(4) $$u_x = - \sigma u + \sigma s u + \sigma s u_s + \sigma s u u_s.$$

This is precisely Equation (23.5) derived there by using quite different methods, and from it may be obtained the usual flux equations for the rod case. It was first pointed out to us by T. E. Harris that the functional equation approach could be applied directly to derivation of the generating function. This is an application of a quite general principle that methods suitable for the derivation of first moments can be used almost unchanged to derive generating functions. From these, relations for the higher moments can be readily obtained. See §51 for another illustration.

28. A Basic Stochastic Functional Equation

We shall now derive a basic stochastic functional equation applicable to the generalized situations described in §26. We introduce the appropriate random variables.

Let

(1) $U(S,S',\eta)$ = random number of particles in state S' reflected from η over all time due to an initial particle in state S impinging on η at time zero. (S and S' may now include information as to the specific location on η.)

(2) $$r(S,\eta) = \begin{cases} 1 & \text{if the particle in state } S \text{ is involved in an interaction in the stratum } (\eta-\Delta,\eta), \\ 0 & \text{otherwise.} \end{cases}$$

(3) $$Z(S;S_1',S_2',\ldots,S_k';\eta) = \begin{cases} 1 & \text{if the result of an interaction of a particle in state } S \text{ with the medium is to produce } k \text{ particles in state } S_1',S_2',\ldots,S_k',\ k = 1,2,3,\ldots, \\ 0 & \text{otherwise.} \end{cases}$$

By the stochastic variables $U^{(i)}, r^{(i)}, Z^{(i)}$ we shall mean respectively any of a denumerable set of variables with the properties described above. Different superscripts will serve merely to distinguish different random variables, and sometimes they will be omitted.

Also, let $Q(S,\eta)$ denote the deterministic change in state caused by passage through the stratum $(\eta-\Delta,\eta)$. By a deterministic change we mean one that occurs by virtue of mere positive change without any interaction necessarily taking place. For example, any dependence of μ on r mentioned in §17 results in such a change.

Finally, we assume that only a finite set of states S is possible. This permits us to use characteristic functions rather than characteristic functionals, and considerably simplifies the discussion.

At the risk of being somewhat redundant, we now discuss the random physical processes which occur. A particle in state S incident on the surface η enters the stratum $(\eta - \Delta, \eta)$. There it may undergo a deterministic transformation converting it from state S to state $Q(S, \eta)$. In addition, it may undergo a stochastic change (collision) producing a random number of particles in a random set of states. Each of these particles acts independently of the others and may emerge from η or be incident upon $\eta - \Delta$. In the latter case the particle is a "source" particle on $\eta - \Delta$, resulting in a random number of particles in a random set of states eventually emerging from $\eta - \Delta$. Each of these reflected particles may undergo deterministic and stochastic transformations in $(\eta - \Delta, \eta)$. Some emerge from η and are counted, others return as source particles into $\eta - \Delta$ and must be followed out again. No processes need be traced to order higher than Δ —that is, to more than one collision in $(\eta - \Delta, \eta)$.

Enumerating these events mathematically, we arrive at the functional equation

(4) $U(S,S',\eta)$

$$= r(S,\eta) \sum_{\{S_1'\}} Z(S;S_1',S_2',\ldots,S_k';\eta)\left[\sum_{i=1}^{k} U^{(i)}(S_i',S',\eta-\Delta)\right]$$

$$+ (1 - r(S,\eta)) \sum_{i=1}^{n} (1 - r^{(i)}(S',\eta))$$

$$+ (1 - r(S,\eta)) \sum_{S_m'}\left[\sum_{i=1}^{n'}\left[r^{(i)}(S_m',\eta)\left\{\sum_{\{S_i''\}} Z^{(j)}(S_m';S_1'',\ldots,S_k'';\eta) \cdot \sum_{p=1}^{k} U^{(p)}(S_p'',\bar{S}',\eta-\Delta)\right\}\right]\right]$$

$$+ w(S,S',\eta),$$

where

$$n = U(Q(S,\eta),S',\eta-\Delta),$$

$$n' = U(Q(S,\eta),S_m',\eta-\Delta),$$

$\bar{S}'$ is such that $S' = Q(\bar{S}',\eta)$,

and $w(S,S',\eta)$ is the contribution from events that have probability $o(\Delta)$. The symbol $\{S_i\}$ means all the subsets of the set of states.

Proceeding as in §27, it is now theoretically possible to derive the flux equation of §27 by taking expected values of (4). It is likely that the direct approach of §26 is really simpler. However, the basic stochastic equation (4) seems of considerable theoretical interest and could well be used for computational purposes in place of a direct Monte Carlo approach.

29. Collision Processes

So far we have not considered transport processes in which the particles interacted with each other, nor processes in which the medium was affected by the transport process. In the sections that follow, we shall consider processes of this nature.

Let us discuss a transport process in a one-dimensional rod in which we allow neutron-neutron interactions, the result being annihilation. To simplify matters, let us suppose that there is no energy dependence, and that collisions occur only between neutrons travelling in opposite directions along the line. As usual, we shall suppose that when fission occurs one neutron is produced in the forward direction and one in the backward direction.

Let

(1) (a) $\sigma\Delta + o(\Delta)$ = the probability that a neutron will interact with a segment of length Δ and produce fission.

(b) $u(y;x,z)$ = the expected number of neutrons per unit time passing an interior point y to the right, as a result of z neutrons per unit time introduced at x (see Fig. 14 below).

(c) $v(y;x,z)$ = the expected number of neutrons per unit time passing an interior point y to the left.

(d) $k(u,v)\Delta + o(\Delta)$ = the expected number of neutrons in a stream of strength u which are annihilated per unit time due to collisions with an opposing stream of strength v, in an interval of length Δ.

Fig. 14

30. Internal Flux Equations

The usual "input—output" analysis yields the relations

$$(1)\qquad \begin{aligned} u(y) &= u(y-\Delta)(1-\sigma\Delta) + u(y-\Delta)\sigma\Delta + v(y)\sigma\Delta \\ &\qquad - \Delta k(u,v) + o(\Delta), \\ v(y) &= v(y+\Delta)(1-\sigma\Delta) + v(y)\sigma\Delta + u(y)\sigma\Delta \\ &\qquad - \Delta k(u,v) + o(\Delta), \end{aligned}$$

where we, at this time, suppress the dependence upon x and z, and write

$$(2)\qquad u(y,x,z) \equiv u(y), \quad v(y,x,z) \equiv v(y).$$

Passing to the limit as $\Delta \to 0$, we are led to the nonlinear system of differential equations

$$(3) \qquad u'(y) = \sigma v - k(u,v),$$
$$v'(y) = -\sigma u + k(u,v).$$

The boundary conditions are

$$(4) \qquad u(0) = 0, \quad v(x) = z,$$

two-point boundary conditions.

31. Discussion

In general, the equations in (30.3) cannot be resolved in terms of elementary transcendents of analysis. Consequently, if we wish to obtain a numerical solution of (30.3) cum (30.4), we must resort to various computational schemes. Although a number of these are available, it cannot be said there are any of automatic application. Questions of this nature are of great difficulty, and perhaps are most easily handled by being bypassed. In the next section we shall approach this problem in a different way.

If we make the assumption that $k(u,v) = buv$, $b > 0$, a certain amount of analysis can be carried out. See [34] for some theoretical and computational results. Henceforth, we assume this form of $k(u,v)$.

32. Reflected and Transmitted Flux

Let us now approach this problem by means of functional equation techniques. Let

(1) $r(z,x)$ = the expected number of neutrons reflected per unit time from a homogeneous bar of length x as a result of having z neutrons incident at x per unit time.

Fig. 15

To evaluate the expected number of neutrons reflected from a bar of length $x + \Delta$ we note, first of all, that some collisions with nucleii may occur immediately when the z neutrons enter the segment $[x, x + \Delta]$. Since each such collision results in a neutron going to the right, $\sigma z\Delta$ particles emerge at $x + \Delta$. Meanwhile, since a neutron is produced going to the left also, the original flux z is not affected by collisions with nucleii. However, this flux is reduced by annihilation by an amount $bzr(z;x)\Delta$ due to the opposing flux out of x. It is also increased by an amount $\sigma r(z;x)\Delta$ due to fission collisions in $[x, x + \Delta]$ made by the flux out of x. Hence there is at x a source of strength $z - bzr(z;x)\Delta + \sigma r(z;x)\Delta$. Finally, the reflected flux due to this source is partially annihilated by interactions with the impinging flux in $[x, x + \Delta]$. Summing up, we are led to the relation

(2) $$r(z;x + \Delta) = \sigma z\Delta + r(z - brz\Delta + \sigma\Delta r(z,x))[1 - bz\Delta] + o(\Delta).$$

By letting Δ tend to zero we find that $r(z;x)$ satisfies the quasilinear first order partial differential equation

(3) $$r_x = \sigma z - bzrr_z + \sigma rr_z - bzr$$

where, as usual, the subscripts indicate partial differentiation. The reflection function $r(z;x)$ also satisfies the initial condition

(4) $$r(z;0) = 0 \quad \text{and} \quad r(0;x) = 0.$$

The Equation (3) specializes, for $b = 0$, to the Riccati equation derived in earlier sections for the reflection coefficient (§4). It may be resolved via characteristic theory [35] or by direct numerical integration, returning essentially to (2). The equations for the characteristics are

(5) $$\frac{dx}{ds} = 1,$$

$$\frac{dz}{ds} = bzr - \sigma r,$$

$$\frac{dr}{ds} = \sigma z - bzr.$$

Since $x = s$, $z = 0$, $r = 0$ is a solution of the system (5) passing through the point $x = z = r = 0$, we find that

(6) $$r(0;x) = 0,$$

as was assumed above on physical grounds.

Once the function $r(z;x)$ has been determined for suitable ranges of z and x, one may reduce the determination of $u(y)$ and $v(y)$, the internal fluxes, to the solution of initial value

problems, as was mentioned earlier. If the incident flux $v(x) = z$ is specified, then the reflected flux is $r(z;x) = u(x)$, so that now both $u(y)$ and $v(y)$ are specified at $y = x$. Through use of Equations (30.3) the functions $u(y)$ and $v(y)$ may now be determined on the entire interval $[0,x]$.

The equations satisfied by the transmitted flux $t(z;x)$, where

(7) $t(z;x)$ = the expected number of neutrons emergent from the end $y = 0$ of a homogeneous bar of length x as a result of having z neutrons per unit time incident on the end $y = x$,

are similarly derived. We have

(8) $$t_x = (\sigma - bz)rt_z$$

along with the boundary conditions

(9) $$t(0;x) = 0, \quad t(z;0) = z.$$

33. Discussion

Numerical solution of the foregoing Equation (32.3), can be obtained either by use of (32.2), by means of conventional techniques, or by means of the characteristics.

In [34] will be found a brief discussion of collision processes of this nature with energy dependence. In the remainder of this paper we consider only processes without particle—particle interaction.

34. Time Dependent Rod Case—Internal Flux

Thus far we have concentrated our attention on the stationary state in dealing with both internal and reflected and transmitted fluxes. In this section we shall obtain the equations for the internal flux in the rod, taking time variation into account. We assume that the rod has all the usual properties, and that neutrons in it travel with speed c. Thus, a time Δ/c is spent in traversing a distance Δ. It is now relatively easy to see that if

(1) $u(y,t)$ = average number of neutrons passing y per second at time t and going to the right;

$v(y,t)$ = average number of neutrons passing y per second at time t and going to the left;

then

(2)
$$u(y + \Delta, t + \tfrac{\Delta}{c}) = u(y,t)(1 - \sigma\Delta) + \sigma\Delta u(y,t) + v(y + \Delta, t)\sigma\Delta + o(\Delta),$$

$$v(y, t + \tfrac{\Delta}{c}) = v(y + \Delta, t)(1 - \sigma\Delta) + \sigma\Delta v(y,t) + u(y,t)\sigma\Delta + o(\Delta),$$

giving in the limit as $\Delta \to 0$ the equations

(3)
$$\frac{1}{c}\frac{\partial u}{\partial t} + \frac{\partial u}{\partial y} = \sigma v,$$

$$\frac{1}{c}\frac{\partial v}{\partial t} - \frac{\partial v}{\partial y} = \sigma u.$$

Equations (3) are subject to the boundary and initial conditions

$$(4) \qquad \begin{aligned} u(0,t) &= 0, \\ v(x,t) &= 1, \\ u(y,0) &= v(y,0) = 0, \end{aligned}$$

for the case of the rod with a unit flux at the right end, $y = x$, imposed at $t = 0$.

This formulation is the classical one. Equation (15.1) already mentioned without discussion is the analogue of (3) for the more complicated geometry. Such equations as (15.1) are readily derived using the principles of this section.

35. Time Dependent Rod Case—Reflected Flux

We now turn to a formulation of the time dependent rod problem using the basic ideas of invariant imbedding. Let us consider a single "trigger" neutron entering the rod at x at time $t = 0$. It is then convenient to introduce

(1) $U(x,t)$ = total number of neutrons reflected from x up to time t due to the one trigger neutron in at x at time $t = 0$.

Clearly

$$(2) \qquad U(x,t) = \int_0^t u(x,s)ds,$$

where u is the function of §34, now subject to the delta function type initial condition. We propose to imbed the rod of length x as usual (see Figure 16).

Fig. 16

It should be noted that this also provides an imbedding in time, and that the important time increment is $2\Delta/c$, representing the time it takes for a particle to cross $[x, x + \Delta]$ in each direction.

We find as usual that there may be an immediate collision in $[x, x + \Delta]$, providing a flux out to the right of $\sigma\Delta$. There is also a single trigger neutron into $[0, x]$, and this enters at time $t = \Delta/c$. At time $s + \Delta/c$ let there be $u(x,s)$ neutrons per second emergent at x. Clearly

(3) $$u(x,s) = \frac{\partial U}{\partial s}(x,s).$$

Some of these neutrons make collisions in $[x, x + \Delta]$. There is surely a flux out of $x + \Delta$ of rate $u(x,s)$. However, half of the fission neutrons return to x at this time. These provide a new source into x, and will contribute to the total flux out during the remaining $t - s$ units of time. Thus

(4) $$U(x, t + \frac{2\Delta}{c}) = \sigma\Delta + U(x,t) + \sigma\Delta\int_0^t u(x,s)U(x,t - s)ds + o(\Delta)$$

giving the equation of mixed differential-integral type

(5) $$\frac{\partial U}{\partial x} + \frac{2}{c}\frac{\partial U}{\partial t} = \sigma + \sigma\int_0^t u(x,s)U(x,t - s)ds,$$

subject to the conditions

(6) $U(x,0) = 0, \quad U(0,t) = 0.$

The system (5) – (6) has been analyzed rigorously (see [45]). The convolution form of the integral term makes possible an explicit analytic representation of the solution when the Laplace transform is used.

36. Modification of Medium during Transport Process

In all that has gone before, we have supposed that the properties of the medium have remained unaltered by the transport process occurring within it. This is, of course, always an approximation of greater or lesser validity.

Two very interesting processes in which interaction with the medium are taken into account are the free boundary problems of hydrodynamics, and the Stefan problems of heat conduction. As a preliminary to an investigation of Stefan-type processes by invariant imbedding techniques, we wish to discuss a one-dimensional transport process in a rod whose length is changing as a function of time.

37. The Physical Process and its Mathematical Formulation

Let us consider a rod which extends from 0 to x at time $t = 0$. The rod grows, or erodes, at a specified rate so that the position of the left end is given by $X_L = f(t)$, $f(0) = 0$, while the right end remains fixed, $X_R = x$. (See the figure below.) A neutron traversing a distance Δ in the rod has, as before, probability $\sigma\Delta + o(\Delta)$ of suffering a

collision with elements of the medium. In the event of a collision, which produces fission, two neutrons emerge, one moving to the left, the other to the right. No neutron can re-enter the rod once having left it, and all neutrons have constant velocity c. A single neutron, the "trigger," enters the rod at x at time $t = s$. We ask for the expected total number of neutrons that emerge at the right end up to time t, denoting this quantity by $U(x,s,t)$.

It must be noted that the condition $(-f'(t)) < c$ for all t is convenient to prevent neutrons from being rather artificially "trapped" in the rod. We shall not discuss interesting problems of this nature here.

To apply the invariant imbedding method, we immerse the original process within the class of all processes indexed by $x > 0$, and then express the relationship between neighboring processes. The left ends are uniformly to obey the same law, $x_L = f(t)$, as that of the original rod.

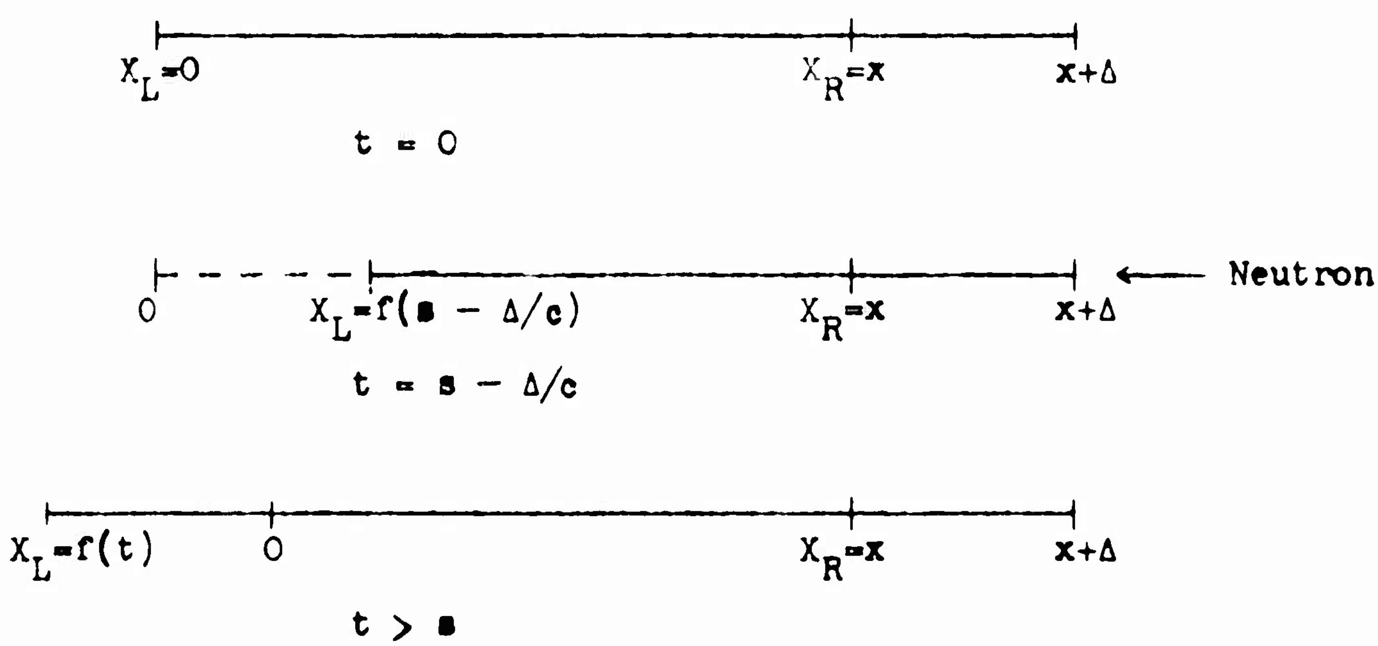


Fig. 17. Neutron transport in a rod of varying length.

Let us now analyze the process. At time $t = s - \Delta/c$ the trigger neutron enters at $x + \Delta$, and may or may not suffer a collision in passing from $x + \Delta$ to x. If it does, a single neutron immediately emerges at the right. In either event, a neutron passes x_R at time $t = s$. This acts as a trigger for the original rod, and produces a flux emergent from x_R at times $t > s$. The expected rate of emergence of such neutrons is given by $u(x,s,t) = \frac{\partial U}{\partial t}(x,s,t)$. Neutrons in this flux may or may not suffer collisions with the rod material in going from x to $x + \Delta$. In either event $U(x,s,t)$ neutrons emerge from $x + \Delta$ by time $t + \Delta/c$. In addition, those neutrons which do make collisions in $(x, x + \Delta)$ at time t', $s < t' < t + \Delta/c$, contribute trigger neutrons at X_R at a rate $\sigma\Delta u(x,s,t') + o(\Delta)$. The resultant flux out of $x + \Delta$ up to time $t + \Delta/c$ is then $\sigma\Delta \int_s^t u(x,s,t')U(x,t',t)dt' + o(\Delta)$. All other processes yield contributions of order $o(\Delta)$. Thus we find

$$
(1) \qquad U(x + \Delta, s - \frac{\Delta}{c}, t + \frac{\Delta}{c}) = \sigma\Delta + U(x,s,t) + \sigma\Delta \int_s^t u(x,s,t')U(x,t',t)dt' + o(\Delta).
$$

Hence, letting $\Delta \to 0$, we obtain the equation

$$
(2) \qquad \frac{\partial U}{\partial x} - \frac{1}{c}\frac{\partial U}{\partial s} + \frac{1}{c}\frac{\partial U}{\partial t} = \sigma + \sigma \int_s^t u(x,s,t')U(x,t',t)dt'.
$$

The conditions imposed on U are

(3) $$U(x,s,t) = 0, \quad s \geq t;$$

$$U(x,s,t) = 0, \quad f(s) = X_R.$$

The first merely states that no neutrons emerge by time t if the trigger enters at a later time, while the second reflects the fact that none can emerge to the right if the rod is of length zero when the trigger neutron impinges.

38. Discussion

Equation (37.2) has the same general structure as that studied in our earlier sections for the case of the rod of fixed length with the neutron entering at $t = 0$. It is not difficult to reduce (37.2) to the simpler equation when $f(t) = 0$. However, the fact that the integral term in (37.2) is no longer of convolution form introduces new complications in studying properties of the solution.

Part III

DIFFUSION THEORY—A LIMITING CASE OF TRANSPORT THEORY

39. Diffusion as a Limiting Process

In previous sections in this paper, we have investigated a variety of simple models of transport theory by means of the functional equation technique of invariant imbedding. Neutrons are mathematically abstracted to be point particles with finite velocities, while fission and scattering are characterized by certain probabilities (cross sections) of branching and reversal or reorientation of direction in the medium within which the process is occurring. In the great proportion of cases we assume no neutron-neutron interaction, and no change in the properties of the medium over time, although we have discussed both of these phenomena to slight extents, §29 and §37.

It is of interest for several reasons, from both the mathematical and physical points of view, to discuss in detail what happens to the various categories of transport equations derived from different applications of invariant imbedding as the velocity of the neutron is allowed to become arbitrarily large with a corresponding increase in the probability of a collision.

This idea is a quite natural one and one that has been pursued by a number of different investigators with different aims in mind. Diffusion theory classically has been regarded as an approximation to the more rigorous (but, of course, not

completely rigorous) transport theory under the assumption of high velocity and small mean free path [40]. Furthermore, passage to the limit in the "telegrapher's equation," a linear partial differential equation of hyperbolic type, has been carried out.

From another direction, the discrete random walk process yields the diffusion equation in the limit. This observation has been made the basis for a considerable amount of analytic and computational effort, centering about the theme of "Monte Carlo" techniques.

Our principal aim here is to study the limits of the non-linear functional equations obtained from the transport processes with finite velocity, e.g. those appearing in §34 and §35, as the velocity increases without bound. In this way, we obtain corresponding results for heat or diffusion processes, where the physical picture is not as clear. Having obtained the equations in this indirect and complex fashion, we can then interpret them in such a way as to be able to derive them directly by invariant imbedding techniques. In all cases, the equations are of the generalized Riccati type which we recognize as characteristic of these processes of mathematical physics, when described in invariant imbedding.

At the present time, we are studying the question of treating Stefan-type diffusion problems by a similar passage to the limit in the equations derived from transport processes with variable boundaries. This is, as might be expected, a complex problem. Some initial results have been given above, §37.

Throughout the sections that follow, we shall use a simple generalization of the idealized one-dimensional rod process treated in the foregoing pages. In the following section, we shall obtain some new equations for the flux within the rod, assuming finite velocities initially. In §41, we derive Fick's law for this simple process. This is important for our purposes, since it is the analysis of this result which suggests the combinations of functions which should be used in the limiting case. In §42, we study the limiting form of the internal flux as the velocity becomes infinite, and in §43 the diffusion process giving rise to the function obtained in this way is analyzed.

We then turn to our primary objective, the passage to the limit of the nonlinear integro-differential equation obtained for the reflected flux in the neutron transport transport case by means of the technique of invariant imbedding. In §45, we show how to obtain the result by direct application of the imbedding technique to the diffusion process.

Throughout this part of the paper, our methods are again largely formal, since we are principally interested in demonstrating the applicability of invariance principles. The existence of relevant limits and the applicability of Laplace transform methods are taken for granted in order to arrive quickly at the desired equations. These questions can be studied in a rigorous fashion, and for the simple mathematical

models considered here, there is little difficulty in carrying out this program. Since, however, we know that the passage to the limit involves a reduction from a hyperbolic partial differential equation to a parabolic partial differential equation, involving inter alia a redundancy in the initial conditions, we can expect some difficulties in the general case. The corresponding study for ordinary differential equations when a limiting value of a parameter results in a drastic change in the order of the equation is of some subtlety. Particularly interesting examples of equations of this nature occur in various hydrodynamical investigations where viscosity plays the role of the parameter which approaches zero; cf. Wasow [41].

40. The Transport Equation

To begin our work it is necessary to write down some transport equations in fairly general form. While some of them are not to be found in the literature, they may be readily derived by the methods of previous sections.

Consider a rod of material which transports neutrons, and let the neutrons have constant velocity c (monoenergetic case). The usual collision processes take place with the probability of a collision in a length Δ of the rod taken to be $\sigma\Delta + o(\Delta)$, where σ is a constant. On the average, $2k$ neutrons emerge from a collision inside the rod, k going to the left and k going to the right. We take the rod to extend from 0 to x (see Fig. 18), and designate the coordinate of an interior point by y.

Fig. 18

To initiate the process, we suppose that there is a time dependent source, $q(t)$ neutrons incident to the left per second at x, and none at the end 0. Finally, we suppose that particles emergent at 0 or x cannot re-enter the rod.

We write

(1) $u(y,t)$ = the average number of neutrons per second passing y at time t and moving to the right,

$v(y,t)$ = the average number of neutrons per second passing y at time t and moving to the left.

Using the methods outlined in §34, it is easily found that

(2)
$$\frac{\partial u}{\partial y} + \frac{1}{c}\frac{\partial u}{\partial t} = \sigma(k-1)u + \sigma k v,$$

$$-\frac{\partial v}{\partial y} + \frac{1}{c}\frac{\partial v}{\partial t} = \sigma k u + \sigma(k-1)v,$$

$$u(0,t) = 0, \quad v(x,t) = q(t), \quad t \geq 0;$$

$$u(y,0) = v(y,0) = 0, \quad 0 \leq y < x.$$

For some purposes it is convenient to talk about the total flux from time 0 to t. We shall consistently use capital letters to indicate quantities integrated over time. Thus

(3) $$U(y,t) = \int_0^t u(y,z)dz,$$

$$Q(t) = \int_0^t q(z)dz,$$

etc. It is easy to see that the integrated quantities satisfy equations identical to (2) with the lower case letters being replaced by capitals.

At times it will be desirable to make clear the type of source in the particular problem under discussion. Hence we shall occasionally write

(4) $$u(y,t;q),$$

$$U(y,t;q)$$

etc., to emphasize the source in question. The source will be deleted when the meaning is clear. In these cases we shall write $u(y,t;q) \equiv u(y,t)$, and so on. In other instances the source may be indicated and the dependence upon y or t left out.

Consider now the case in which the source consists of a single "trigger" neutron at $t = 0$. Thus, formally, $q(t) = \delta(t)$, where δ is the Dirac delta function. We focus attention on the particles reflected from the rod at x, writing $r(x,t;\delta)$ for the number emergent per second, and $R(x,t,\delta)$ for the total number emergent up to time t. Clearly

$$(5) \qquad r(x,t;\delta) = u(x,t;\delta),$$
$$R(x,t;\delta) = U(x,t;\delta).$$

However, it is again well to regard the x in the arguments of r and R as referring to the <u>length</u> of the rod rather than to the coordinates of the end point of the rod. With this rather subtle distinction in mind one then finds, proceeding as before (§35),

$$(6) \qquad \frac{\partial R(\delta)}{\partial x} + \frac{2}{c}\frac{\partial R(\delta)}{\partial t} = \sigma k + 2\sigma(k-1)R(\delta)$$
$$+ \sigma k \int_0^t r(x,z;\delta)R(x,t-z;\delta)dz,$$
$$R(x,0;\delta) = R(0,t;\delta) = 0.$$

Notice that this characterizes the reflected flux in a fashion <u>independent of the internal fluxes</u>.

For the corresponding case in which there is a source $q(t)$, we note that the fundamental physical process is additive, as a consequence of our tacit assumption that there are no interactions between neutrons passing in opposite directions, we can write

$$(7) \qquad R(x,t;q) = \int_0^t q(z)R(x,t-z;\delta)dz.$$

To find an equation satisfied by $R(x,t;q)$, we utilize the Laplace transform, writing

$$(8) \qquad R(x,s) = \int_0^\infty e^{-st}R(x,t)dt,$$

with a consistently similar notation for transforms of other functions. Then, from (6), with $q = \delta$,

$$(9) \qquad \frac{dR_L(\delta)}{dx} + \frac{2}{c}\, sR_L(\delta) = \frac{\sigma k}{s} + 2\sigma(k - 1)R_L(\delta) + \sigma k s R_L{}^2(\delta),$$

$$R_L(0,s;\delta) = 0.$$

From (7),

$$(10) \qquad R_L(x,s;q) = q_L(s)R_L(x,s;\delta).$$

Hence,

$$(11) \qquad \frac{dR_L(q)}{dx} + \frac{2}{c}\, sR_L(q) = \frac{\sigma k}{s}\, q_L + 2\sigma(R - 1)R_L(q)$$

$$+ \sigma k s R_L(q)R_L(\delta),$$

which leads back to

$$(12) \qquad \frac{\partial R(q)}{\partial x} + \frac{2}{c}\frac{\partial R(q)}{\partial t} = \sigma k Q(t) + 2\sigma(k - 1)R(q)$$

$$+ \sigma k \int_0^t r(x,z;\delta)R(x,t - z;q)dz,$$

$$R(0,t;q) = R(x,0;q) = 0.$$

This clearly reduces to (6) when $q(t) = \delta(t)$.

We shall derive one other special case of (12), corresponding to the case when $q(t) = 1$. While conceptually this may be a bit more difficult to consider than the single trigger neutron case, it has the mathematical advantage of avoiding the δ-function. For this type of source we write the integrated flux as $R(x,t;1)$ or $R(1)$ and (12) becomes

$$(13) \qquad \frac{\partial R(1)}{\partial x} + \frac{2}{c}\frac{\partial R(1)}{\partial t} = \sigma kt + 2\sigma(k-1)R(1) + \sigma k \int_0^t r(x,z;\delta)R(x,t-z;1)dz.$$

But, from (7),

$$(14) \qquad R(x,t;1) = \int_0^t R(x,t-z;\delta)dz.$$

Then we easily find

$$(15) \qquad \frac{\partial R(1)}{\partial x} + \frac{2}{c}\frac{\partial R(1)}{\partial t} = \sigma kt + 2\sigma(k-1)R(1) + \sigma k \int_0^t r(x,z;1)r(x,t-z;1)dz,$$

$$R(0,t;1) = R(x,0;1) = 0.$$

41. Fick's Law

If we subtract the second equation of (40.2) from the first we obtain

$$(1) \qquad \frac{\partial}{\partial y}(u+v) + \frac{1}{c}\frac{\partial}{\partial t}(u-v) = -\sigma(u-v).$$

For large c, we expect the second term on the left to be small. Hence we formally obtain the relation

$$(2) \qquad \frac{\partial}{\partial y}(u+v) = -\sigma(u-v)$$

in the "limit of large velocity." Equation (2) is ordinarily referred to as Fick's Law [40], which states that the net flux is proportional to the gradient of the concentration and in the opposite direction.

42. The Limiting Case Obtained Directly

To obtain preliminary results we take Laplace transforms of (40.2). Thus, using the notation introduced in (40.7),

$$(1)\qquad \frac{du_L}{dy} + \frac{s}{c}\,u_L = \sigma(k-1)u_L + \sigma k v_L,$$

$$-\frac{dv_L}{dy} + \frac{s}{c}\,v_L = \sigma k u_L + \sigma(k-1)v_L,$$

$$u_L(0,s) = 0, \quad v_L(x,s) = q_L(s).$$

After rather extensive but rudimentary calculations, we arrive at the relations

$$(2)\qquad u_L(y,s) = \frac{k\sigma q_L(s)\,\sinh \lambda y}{\left\{\lambda \cosh \lambda x + \left(\frac{s}{c} + (1-k)\sigma\right)\sinh \lambda x\right\}},$$

$$v_L(y,s) = \frac{q_L(s)\left\{\lambda \cosh \lambda y + \left(\frac{s}{c} + (1-k)\sigma\right)\sinh \lambda y\right\}}{\left\{\lambda \cosh \lambda x + \left(\frac{s}{c} + (1-k)\sigma\right)\sinh \lambda x\right\}},$$

where

$$(3)\qquad \lambda^2 = \left(\frac{s}{c}\right)^2 + \frac{2(1-k)\sigma}{c}\,s + \sigma^2(1-2k).$$

We now choose $k = 1/2$, which means physically that an average collision gives rise to one neutron. This choice eliminates the last term in (3). Since we seek a diffusion type equation, we let $c \longrightarrow \infty$, which is to say, we allow the velocity to become infinite. Clearly, to preserve the process we must then require that $\sigma \longrightarrow \infty$ in such a way that $\lim\ c/\sigma = D$, a constant. Hence, from what has proceeded, $\lim \lambda = \sqrt{s/D}$.

(It should be noted that a somewhat more general result could have been obtained by requiring, instead of $k = 1/2$,

that $\lim \sigma^2(1 - 2k) = \alpha$. By so doing we could have accounted for cases of absorption or fission. To do this here would merely complicate the ensuing calculations.)

Bearing (50.2) in mind, we set

$$(4) \qquad j_L(y,s) = \sigma(u_L(y,s) - v_L(y,s)),$$

$$j_{0,L}(y,s) = \lim_{\sigma \to \infty} j_L(y,s).$$

Let us consistently reserve the subscript zero to refer to quantities in the limit as $c \to \infty$.

We then discover that

$$(5) \qquad j_{0,L}(y,s) = -\lim_{\sigma \to \infty} \frac{\sigma q_L(s)\lambda \cosh \lambda y}{\left\{\lambda \cosh \lambda x + (\frac{s}{c} + \frac{\sigma}{2})\sinh \lambda x\right\}}$$

$$= -2q_L(s) \frac{\sqrt{D^{-1}s} \cosh (y\sqrt{D^{-1}s})}{\sinh (x\sqrt{D^{-1}s})} .$$

43. A Classical Diffusion Problem

We now seek an ordinary diffusion problem which gives rise to the limiting expression found in (41.5). It is readily verified that if $\theta(y,t)$ is implicitly determined by the relations

$$(1) \qquad D\frac{\partial^2\theta}{\partial y^2} = \frac{\partial\theta}{\partial t}, \quad \theta(0,t) = 0, \quad \theta(x,t) = 2q(t), \quad \theta(y,0) = 0,$$

then, explicitly,

$$(2) \qquad \theta_L(y,s) = \frac{2q_L(s)\sinh(y\sqrt{D^{-1}s})}{\sinh (x\sqrt{D^{-1}s})},$$

and

$$(3) \qquad \frac{d\Theta_L}{dy} = 2q_L(s)\sqrt{D^{-1}s}\,\frac{\cosh(y\sqrt{D^{-1}s})}{\sinh(x\sqrt{D^{-1}s})} .$$

We may summarize our results thus far as follows:

If we consider the transport problem formulated in (40.2) in the limiting case where $c \to \infty$, $c/\sigma \to D$, with $k = 1/2$, then the problem is formally equivalent to the classical diffusion problem (1). The quantity $\lim_{\sigma\to\infty} (u(y,t) + v(y,t))$ may be identified with $\Theta(y,t)$, while $\lim_{\sigma\to\infty} \sigma(u(y,t) - v(y,t))$ corresponds to $-\partial\Theta/\partial y$.

It is possible to identify $\Theta(y,t)$ with the total neutron flux (see [40]) although the diffusion may refer as well to heat or material concentration. The fact that a source of $2q(t)$ is required as part of the initial conditions in the problem (1) may be rather puzzling until one notes from (42.2) that, formally, both $u(x,t)$ and $v(x,t)$ approach $q(t)$ as $c \to \infty$.

44. The Reflected Flux

Let us now turn to Equation (40.15) and try to carry out the same type of passage to the limit. It is clear that we must begin by investigating the quantity

$$(1) \qquad H(x,t;q) = \sigma\{R(x,t;q) - Q(t)\} ,$$

which reduces to $\sigma\{R(x,t;1) - t\}$, when $q(t) = 1$. Thus,

$$(2) \qquad R(1) = \frac{H(1)}{\sigma} + t,$$

$$r(1) = \frac{h(1)}{\sigma} + 1.$$

Substituting these in (40.15) with $k = 1/2$, we find

$$(3)\qquad \frac{1}{\sigma}\frac{\partial H(1)}{\partial x} + \frac{2}{c}\left(\frac{h(1)}{\sigma} + 1\right) = \frac{\sigma t}{2} - \sigma\left(\frac{H(1)}{\sigma} + t\right)$$
$$+ \frac{\sigma}{2}\int_0^t \left\{\frac{h(x,z;1)}{\sigma} + 1\right\}\left\{\frac{h(x,t-z;1)}{\sigma} + 1\right\} dz$$

From this we readily get

$$(4)\qquad \frac{\partial H(1)}{\partial x} + \frac{2\sigma}{c}\left(\frac{h(1)}{\sigma} + 1\right) = \frac{1}{2}\int_0^t h(x,z;1)h(x,t-z;1),$$

$$H(x,0;1) = 0, \quad H(0,t;1) = -\sigma t.$$

Passing to the limit as in §43 we get (at least formally)

$$(5)\qquad \frac{\partial H_0(1)}{\partial x} + 2D^{-1} = \frac{1}{2}\int_0^t h_0(x,z;1)h_0(x,t-z;1)dz,$$

$$H_0(x,0;1) = 0, \quad H_0(0,t;1) = -\infty;$$

where $H_0(x,t;q) = \lim_{\sigma\to\infty} H(x,t;q)$, etc., as agreed. That (5) is the correct limiting form may be established by a Laplace transform argument similar to that of the last section. We omit the details.

It is of some interest to evaluate H_0. This may be done by solving (5), of course. However, it is easier for us to note from (42.5) that

$$(6)\qquad h_{0,L}(x,s;q) = -2q_L(s)\frac{\sqrt{D^{-1}s}\,\cosh\,(x\sqrt{D^{-1}s})}{\sinh\,(x\sqrt{D^{-1}s})}$$

$$= -\frac{2}{\sqrt{sD}}\coth\,(x\sqrt{D^{-1}s}),$$

when $q(t) = 1$. We find

$$(7) \qquad h_0(x,t;1) = -\frac{2}{\sqrt{\pi t D}}\left\{1 + 2\sum_{n=1}^{\infty} e^{-\frac{x^2n^2}{tD}}\right\}$$

$$= -\frac{2}{x}\,\theta_0\left(\frac{1}{2},\frac{t}{Dx^2}\right),$$

where θ_0 is a theta function.

The analogue of (5) may be derived easily for the case in which there is an arbitrary source $Q(t)$. The result is

$$(8) \qquad \frac{\partial H_0(q)}{\partial x} + 2D^{-1}q(t) = \frac{1}{2}\int_0^t h_0(x,z;1)h_0(x,t-z;q)dz,$$

$$H_0(x,0;q) = 0, \quad H_0(0,t;q) = -\infty .$$

We now readily see the following result:

<u>If we consider the transport problem formulated in</u> (40.2) <u>in the limiting case then the quantity</u> $H_0(x,t;q)$ <u>is formally equivalent to the quantity</u> $-\frac{\partial}{\partial y}\int_0^t \theta(y,z)dz\Big|_{y=x}$ <u>where</u> θ <u>is defined by</u> (43.1). <u>Further</u> $H_0(q)$ <u>satisfies</u> (8) <u>with</u> $h_0(1)$ <u>given by</u> (5).

45. A Direct Invariant Imbedding Approach in Diffusion Theory

The equations thus far obtained are not new, though our approach to them may be somewhat novel. To conclude our work here we shall present a method of obtaining (44.8) by invariant imbedding techniques without venturing outside the confines of ordinary diffusion theory. The method described holds promise of being applicable in much more complicated diffusion processes than that described here, and, in particular, may eventually yield new formulations of Stefan-type problems.

To be consistent in our viewpoint, we now think of $\phi(y,t)$ as the density of neutrons at y at time t. Then the net neutron current density $i(y,t)$ is provided by Fick's Law, in the ordinary diffusion approach [40],

(1) $$i(y,t) = -D\frac{\partial}{\partial y}\phi(y,t).$$

The conservation of particles (since there is no internal production when $k = 1/2$) requires in any interval (a,b) of the rod

(2) $$i(b,t) - i(a,t) = -\frac{\partial}{\partial t}\int_a^b \phi(y,t)dy.$$

Let us write, for the net current emerging from our rod of length x, $k(x,t)$. Here, again, while it is true that $k(x,t) = i(x,t)$ we choose to regard the x in the function k as referring to the <u>length</u> of the rod. Thus $k(x + \Delta,t)$ is the net current emergent from a rod of length $x + \Delta$, source $2q(t)$ at $(x + \Delta)$, other initial and boundary conditions being as before.

We now try to express $k(x + \Delta,t)$ in terms of $k(x,t)$. Applying (2) to the rod of length $x + \Delta$ we find

(3) $$k(x + \Delta,t) - i(x,t) = -\frac{\partial}{\partial t}\int_x^{x+\Delta} \phi(y,t)dy,$$

or, integrating over time,

(4) $$K(x + \Delta,t) - I(x,t) = -\int_x^{x+\Delta} \phi(y,t)dy.$$

We now seek expressions for $I(x,t)$ and ϕ. To find $I(x,t)$ we note that we have thus far disregarded the part of the rod from 0 to x. By the continuity conditions imposed by diffusion theory, we know that $I(x,t)$ is merely the current out of x due to the source $\phi(x,t)$ imposed. Let us suppose that a steady source of unit strength produces a current out of the rod of $p(x,t)$. Then a source $\phi(x,t)$ will produce an integrated current

$$(5) \qquad I(x,t) = \int_0^t p(x,t-z)\phi(x,z)dz.$$

(This is just Duhamel's Principle [35]).

As yet we have not used (1). From it we find

$$(6) \qquad \phi(x,t) = \frac{\Delta}{D} k(x+\Delta,t) + 2q(t) + o(\Delta).$$

Substituting (5) and (6) in (4), we obtain

$$(7) \qquad K(x+\Delta,t) = \int_0^t p(x,t-z)\left\{\frac{\Delta}{D} k(x+\Delta,z) + 2q(z)\right\} dz$$

$$- 2\Delta q(t) + o(\Delta).$$

But, by Duhamel's Principle,

$$(8) \qquad \int_0^t p(x,t-z)2q(z)dz = K(x,t).$$

Thus

$$(9) \qquad \frac{\partial K}{\partial x} + 2q(t) = \frac{1}{D}\int_0^t p(x,t-z)k(x,z)dz.$$

This agrees with (44.8) upon identifying k with $Dh_0(q)$ and p with $\frac{D}{2} h_0(1)$, the factor 1/2 occurring because p is the current due to a unit source, while h_0 is obtained from a source of strength 2.

It is clear that

(10) $$K(x,0) = 0.$$

To find $K(0,t)$ we note from (6) that

$$\phi(0,t) = 0 = \frac{\Delta}{D} k(\Delta,t) + 2q(t) + o(\Delta),$$

so that for $Q(t) > 0$,

(11) $$K(0,t) = -\infty.$$

Clearly, in case $q = 1$, we have

(12) $$\frac{\partial P}{\partial x} + 2 = \frac{1}{D}\int_0^t p(x,t - z)p(x,z)dz,$$

$$P(x,0) = 0, \quad P(0,t) = -\infty.$$

Part IV

RANDOM WALK AND MULTIPLE SCATTERING

46. Random Walk

We now wish to apply invariant imbedding techniques to the study of random walk processes. Subsequently, we shall consider more general processes of this nature, equivalent to multiple scattering processes.

Consider the finite one-dimensional lattice consisting of the integer values between a and b along the real line, as indicated below.

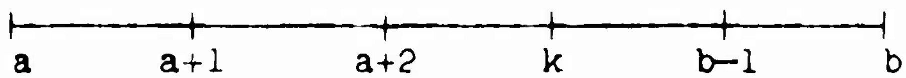


Fig. 19

A particle jumps from lattice-point to lattice-point in accordance with the following law. When at k, there is a probability $q(k)$ of moving one unit to the right and a probability $p(k) = 1 - q(k)$ of moving one unit to the left.

We wish to determine the probability that the particle, starting at k, hits the barrier at a before it hits the barrier at b. The process ends as soon as the particle lands at a or b--hence, the name "absorbing barriers."

This is an extension of the classical "gambler's ruin" process in which $p(k) = q(k) = 1/2$ for $a < k < b$. This particular case can be treated in a very elegant fashion by means of Wald's "fundamental identity." See [36] for generalizations to the case of dependent steps. Another extension is the "game of survival," [18].

The classical approach, also based upon the use of recurrence relations, proceeds as follows, [37]. Let

(1) $u(k)$ = the probability that a particle starting at k lands at a before it lands at b.

Then, considering what happens as a result of the first step, for $a < k < b$,

$$(2) \qquad u(k) = p(k)u(k-1) + q(k)u(k+1),$$

with the two-point boundary conditions

$$(3) \qquad u(a) = 1, \quad u(b) = 0.$$

We thus face the problem of solving a system of linear equations, something we wish to avoid if possible. In what follows we shall attack these problems by a quite different method.

47. Invariant Imbedding Approach

The observation that the desired probability, $u(k)$, is a function of the endpoints a and b, as well as of k,

keys our approach. Hence, we should write $u(k,a,b)$ to signify this dependence.

Invariant imbedding, as we have repeatedly stated, capitalizes upon this dependence. In place of considering a and b to be constants, we consider them to be parameters of equal importance with k, which means that in place of treating an individual random walk process, we investigate simultaneously an entire family of processes. The individual problem is then analyzed in terms of its relation to contiguous members of the family. In this way, we hope to construct a bridge between particular elements of the family of quite simple analytic structure and the processes of interest to us.

Let us then keep one endpoint fixed, say b, and regard u as a function of a and k. To make this dependence explicit, let us introduce the new function

(1) $f(a,k)$ = the probability that a particle starting at k, $a \le k \le b$, will reach a before reaching b.

Clearly $f(a,k) = u(k;a,b)$.

To obtain the required relation between contiguous elements, we use the simple geometric fact that a particle starting at k, and moving one unit in either direction at each stage, must hit $a + 1$ before it can hit a. This is analogous to the stratification technique we used in the discussion of neutron transport and multiplication. Having

reached $a + 1$, the particle must then reach a before b, if this is to be the case for the original process.

Translating these remarks into algebraic relations, using the elementary rules of probability theory, we have

$$(2) \qquad f(a,k) = f(a + 1,k)f(a,a + 1).$$

Iterating this relation, we have

$$(3) \qquad f(a,k) = f(a,a + 1)f(a + 1,a + 2)\cdots f(k - 1,k).$$

an interesting representation for solutions of a Jacobi system of equations of the type appearing in (37.2).

We have deliberately stressed the word "elementary" in the foregoing discussion, since we can employ similar methods based upon other concepts of probability to discuss other kinds of equations. For other methods of treating Jacobi equations, see [38].

48. The Function $f(a,a + 1)$

To answer our original question, that of determining the value of $f(a,k)$, it remains to evaluate the functions of one variable

$$(1) \qquad g(a) = f(a,a + 1),$$

defined for $a \leq b - 1$. Clearly $g(b - 1) = 0$.

Reverting to the description of the original process, we obtain the relation

(2) $$f(a,a+1) = p(a+1) + q(a+1)f(a,a+2).$$

Using (47.2), we have

(3) $$f(a,a+2) = f(a+1,a+2)f(a,a+1).$$

Combining these two expressions, we obtain the recurrence relation

(4) $$g(a) = \frac{p(a+1)}{1 - q(a+1)g(a+1)}.$$

Since, as noted above, $g(b-1) = 0$, we have a simple inductive determination of $u(a)$ for $a \leq b-1$.

49. An Alternative Derivation

The foregoing result can be derived in a way which emphasizer its physical significance and its connection with previous work on neutron diffusion. Toward this end, let us consider the following scattering problem. A rod extending from a to b has the property that if a particle is at the position k, there is probability $p(k)$ that it will be scattered to $k-1$, and probability $q(k) = 1 - p(k)$ that it will be scattered to $k+1$. A particle is placed at the end a, and we wish to determine the probability that it will be "back-scattered" (reflected) from a, over all time, rather than be "forward-scattered" (transmitted) through the end b.

We imbed this process within the class of processes with "trigger" particles placed at the end ℓ of rods extending from ℓ to b, with $\ell = b, b-1, \ldots,$ and then write a functional equation interconnecting these processes.

Let us define the function $g(a)$ directly

(1) $g(a)$ = the probability that over all time a particle at $a + 1$ will be backscattered to a by the rod extending from $a + 1$ to b, rather than be forwardscattered at b from the rod.

Observe next that with the particle initially at the position $a + 1$, there is probability $p(a + 1)$ that it will be scattered directly to the point a. On the other hand, if it is scattered initially to the right to $(a + 2)$, then by definition there is probability $g(a + 1)$ that it will eventually be back-scattered from the rod $(a + 2, b)$ to the point $a + 1$, from which it may be scattered to the point a. Should, however, it once again be scattered to the right, to the point $(a + 2)$, there is once again probability $g(a + 1)$ that it will eventually reach the point $a + 1$, and so on. In this way we see that

(2) $$g(a) = p(a + 1) + q(a + 1)g(a + 1)p(a + 1) + q(a + 1)g(a + 1)q(a + 1)g(a + 1)p(a + 1) + \cdots,$$

which, upon summing the geometric series on the right hand side, leads to the equation

(3) $$g(a) = \frac{p(a + 1)}{1 - q(a + 1)g(a + 1)}.$$

This id Equation (48.4).

The method that we have used in deriving Equation (48.2) of (3) corresponds abstractly to the method used by Ambarzumian [29] in discussing diffuse reflection from a foggy medium, a process we shall discuss below, and to the method used above in handling some neutron transport processes.

Similarly, the discussion in §47 may be reinterpreted to yield the flux scattered from the end a of a rod as a result of an internal source of particles.

50. Expected Sojourn

Let us now introduce the function

(1) $w(a,k)$ = the conditional expected time required for the particle to reach a before reaching b, starting from k, assuming a unit step takes unit time.

By this we mean the expected time required to reach a, under the assumption that a is reached before b. Then, the same reasoning as above yields the relation

$$w(a,k) = w(a + 1,k) + w(a,a + 1). \tag{2}$$

To obtain an analytic expression for $w(a,a + 1)$, we combine the two expressions

$$w(a,a + 1) = p(a + 1) + q(a + 1)[w(a,a + 2) + 1], \tag{3}$$

$$w(a,a + 2) = w(a + 1,a + 2) + w(a,a + 1).$$

The result is

(4) $$w(a, a+1) = \frac{1}{p(a+1)} + \frac{q(a+1)}{p(a+1)} w(a+1, a+2).$$

Iteration yields the infinite series

(5) $$w(a, a+1) = \frac{1}{p(a+1)} + \frac{q(a+1)}{p(a+2)p(a+1)} + \frac{q(a+1)q(a+2)}{p(a+3)p(a+2)p(a+1)} + \cdots,$$

with the convention that the series terminates if b is finite.

51. Characteristic Functions

As we have pointed out above, whenever an expected value can be determined, the same techniques yield relations for generating functions. Let

(1) $$y(a, k, s) = E(e^{isz}),$$

where $z = z(a, k)$ is the random variable equal to the time spent by the particle in going from k to a, without ever hitting b.

Since

(2) $$z(a, k) = z(a+1, k) + z(a, a+1),$$

we have the functional equation

(3) $$y(a, k, s) = y(a+1, k, s)y(a, a+1, s).$$

It is now not hard to show that

$$(4) \qquad y(a,a+1) = p(a+1)e^{is} + q(a+1)e^{is}y(a,a+2),$$

$$y(a,a+2) = y(a+1,a+2)y(a,a+1).$$

From these we obtain the recurrence relation

$$(5) \qquad y(a,a+1) = \frac{p(a+1)e^{is}}{1 - q(a+1)e^{is}y(a+1,a+2)},$$

which can be used to obtain higher moments, [39].

52. More General Random Walk Processes

Similar methods can be applied to random walks which allow steps of different units at each stage. Abstractly, these methods will be equivalent when vector-matrix notation is introduced.

53. Multiple Scattering

In this part of the paper, we wish to consider two processes of particular interest. The first concerns a one-dimensional random walk in which the energy of the particle changes as a result of its wandering, while the second pertains to a two-or-three-dimensional random walk process in which the direction of motion changes as a result of each collision.

Both of these can, in discrete form, be considered to be particular cases of a process of the following type:

"A particle in state i, $i = 1,2,\dots,N$, can occupy any of the lattice points k between a and b. Let

(1) $p_{ij}(k)$ = the probability that a particle at k in state i will go one unit to the left, and arrive in state j, $i,j = 1,2,\ldots,N$,

$q_{ij}(k)$ = the probability that a particle at k in state i will go one unit to the right, and arrive in state j, $i,j = 1,2,\ldots,N$."*

Let us then define the N^2 functions

(2) $u_{ij}(a,k)$ = the probability that a particle starting at k in state i will hit a in states j before reaching b in any state.

Proceeding as in the foregoing sections, we obtain the relation

$$(3) \qquad u_{ij}(a,k) = \sum_m u_{im}(a+1,k)u_{mj}(a,a+1).$$

Consequently, if we introduce the matrix function

$$(4) \qquad U(a,k) = (u_{ij}(a,k)),$$

we derive the basic relation

$$(5) \qquad U(a,k) = U(a+1,k)U(a,a+1),$$

the analogue of (47.2). Once again, we see that the problem has reduced to a determination of a function of a alone, $U(a,a+1)$.

---

*It is convenient here to reverse the index order as compared to previous usage (see §8).

54. Determination of $U(a, a+1)$

Proceeding as before, we have

(1) $$u_{ij}(a, a+1) = p_{ij}(a+1) + \sum_m q_{im}(a+1) u_{mj}(a, a+2),$$

or, if $G(a) = (u_{ij}(a, a+1))$, $P(a) = (p_{ij}(a))$, $Q(a) = (q_{ij}(a))$,

(2) $$G(a) = P(a+1) + Q(a+1)U(a, a+2).$$

Using (53.2), we obtain the relation

(3) $$U(a, a+2) = U(a+1, a+2)U(a, a+1).$$

Using this in (2), we have

(4) $$G(a) = P(a+1) + Q(a+1)G(a+1)G(a),$$

or

(5) $$G(a) = \left[I - Q(a+1)G(a+1)\right]^{-1} P(a+1).$$

Since $G(b-1) = 0$, once again we have a direct iterative technique for determining $G(a)$, and thus $U(a, x)$.

55. Discussion

It is clear that in the same way we can obtain multidimensional analogues of the results for the expected sojourn and generating function.

Turning from the analytic aspects, let us examine the computational aspects. Approaching the problem along conventional lines, we obtain a system of linear equations of the form

(1) $$u_{ij}(k) = \sum_m p_{im}u_{mj}(k-1) + \sum_m q_{im}(k)u_{mj}(k+1).$$

Keeping j fixed, we have a system of order $N(b-a)$. If $N = 10$, and $b - a = 100$, this is order 1000, a respectable and even formidable number, even in the light of modern devices.

Using the technique described above, the solution is made to depend upon the inversion and repeated multiplication of 10×10 matrices, a complicated, but far more feasible process.

56. Time-dependent Processes

Let us now consider the one-dimensional random walk process in which each stage consumes one time unit. Let

(1) $u(a,k,t)$ = the probability of going from k to a in time t, without ever hitting b.

As we shall see, we derive equations completely analogous to those exhibited above for the generating function

(2) $$F(a,k,t,r) \equiv F(a,k) = \sum_{t=0}^{\infty} u(a,k,t)r^t.$$

As in the previous sections, we obtain the fundamental relation

(3) $$u(a,k,t) = \sum_{s=0}^{t} u(a+1,k,s)u(a,a+1,t-s),$$

and once again derive the fundamental relation

(4) $$F(a,k) = F(a+1,k)F(a,a+1).$$

Furthermore,

$$(5)\qquad u(a,a+1,t) = p(a+1)\delta(1,t) + q(a+1)u(a,a+2,t-1),$$

for $t \geq 1$, where

$$(6)\qquad \delta(1,t) = 1, \quad t = 1,$$
$$= 0, \quad t \neq 1.$$

Thus, multiplying (5) by r^t and summing over t,

$$(7)\qquad F(a,a+1) = p(a+1)r + q(a+1)rF(a,a+2).$$

From here on the argument proceeds as before. The final result is

$$(8)\qquad F(a,a+1) = \frac{p(a+1)r}{1 - q(a+1)rF(a+1,a+2)}.$$

Equation (7) can be derived directly making use of the properties of the process and of generating functions. It should be compared with (51.5).

Part V

RADIATIVE TRANSFER

57. Introduction

In these last few sections we shall discuss a problem arising in the field of radiative transfer. Abstractly, such cases are equivalent to appropriate neutron transport problems, and therefore the material appearing here could very well have been placed in earlier sections. However, since it was in the solution of problems of this genre that Ambarzumian [29] first successfully used his invariance principle and here, too, that Chandrasekhar developed his extensive generalization [30] it seems fitting that we leave these problems in their original setting. Our discussion follows that of [42] in which the principle of invariant imbedding was first sketched.

58. The Physical Model

Assume that parallel rays of light of uniform intensity are incident on an inhomogeneous slab composed of a substance which absorbs and scatters light. Our objective is to determine the intensity of the diffusely reflected light as a function of the incident light, the properties of the slab, and the angle of the emerging rays.

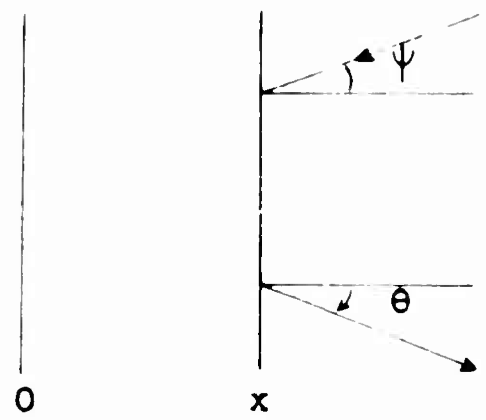


Fig. 20

Cross section of slab with
incident and reflected rays.

We shall assume the slab has the following absorption and scattering properties.

(1) In traversing a distance d in the slab a portion of a beam I is reduced to intensity $I(1 - ad) + o(d)$. A fraction λ of the intercepted beam is reradiated, while a fraction $1 - \lambda$ is permanently lost (absorbed). The quantities λ and a may be dependent upon the distance from an edge of the slab.

(2) Radiation is scattered isotropically.

In the light of our previous work, it is most convenient to consider the light radiation as composed of photons; particles, then, which behave, for our purposes, just as neutrons do.

We must note, too, that in reality not only the angles ψ and θ (Fig. 20) arise but also the corresponding azimuthal angles. The latter may be neglected in our analysis because of the symmetry of the problem.

We define a reflection coefficient $R(x,\psi,\theta)$, giving the intensity of radiation reflected in direction θ per unit area on the face of the slab due to a beam of unit intensity incident at angle ψ, the thickness of the slab being x. Otherwise put, R is the number of photons per unit time out of a unit area on the slab at angle θ, due to a unit flux (one photon per unit area per unit time) impinging at angle ψ.

It is now easy to write down the equations for R, either using directly the fundamental principles we have developed, or applying the general flux equation (26.2). We find, recalling that integrations over the azimuthal angles are necessary, even though R is independent of them,

$$
\begin{aligned}
(1) \qquad \frac{\partial R}{\partial x} = {} & \frac{a(x)\lambda(x)}{4\pi\cos\psi} - a(x)\left(\frac{1}{\cos\theta} + \frac{1}{\cos\psi}\right)R(x,\psi,\theta) \\
& + \frac{a(x)\lambda(x)}{2\cos\psi}\int_0^{\pi/2} R(x,\psi',\theta)\sin\psi' d\psi' \\
& + \frac{a(x)\lambda(x)}{2}\int_0^{\pi/2} R(x,\psi,\theta')\frac{\sin\theta'}{\cos\theta'}\, d\theta' \\
& + a(x)\lambda(x)\pi\int_0^{\pi/2} \frac{\sin\theta'}{\cos\theta'} R(x,\psi,\theta')d\theta' \int_0^{\pi/2} R(x,\psi',\theta)\sin\psi' d\psi'.
\end{aligned}
$$

59. Comparison with the Results of Ambarzumian

Equation (58.1) is considerably more general than the original result of Ambarzumian, since that writer considered a semi-infinite slab, with $a = 1$ and λ constant. Our result should hence reduce to his when we eliminate the x dependence and set $\partial R/\partial x = 0$. The reader will find, however, that the equations still differ considerably.

The reason for this apparent discrepancy lies in the way we have chosen to measure flux throughout this paper. While classically flux is measured in terms of the number of particles per unit time crossing a unit area normal to the direction of the particle, we have chosen instead to talk in terms of the number per unit time through a unit area on the (geometric) surface through which the particles are passing.

A bit of philosophy may be appropriate. The transport equation for the flux of particles internal to a body ordinarily is quite independent of the boundaries of the medium itself. The geometry is brought in through the auxiliary boundary conditions. Thus a person in outer space, with no frame of reference, would rather naturally measure flux in the classical way.

The equations of invariant imbedding, however, depend deeply and inherently upon the boundaries of the body under consideration. It therefore seems natural to define the flux with direct reference to those boundaries. We have found this the easier way conceptually.

In any event it is possible to convert from one definition of flux to the other without great effort. Consider the case of §58, and let us define $I(x,\psi,\theta)$ as the reflected intensity in the classical sense: $I(x,\psi,\theta)$ is the number of photons reflected from x travelling in direction θ per unit time through a unit area normal to that direction due to one photon incident on x per unit time per unit area normal to the direction ψ. Then it is easy to see that

$$\text{(1)} \qquad I(x,\psi,\theta) = R(x,\psi,\theta)\left(\frac{\cos\psi}{\cos\theta}\right).$$

Using the foregoing transformation, we obtain Ambarzumian's equation.

Part VI

SUMMARY

60. Review of Basic Techniques

Having covered some quite diverse parts of mathematical physics, we feel that it is important to state to the reader what our basic ideas and objectives have been, and what have been the methods we have employed toward obtaining these goals.

We start with the fact that any physical process can be described in a variety of different ways, leading to a number of different analytic paraphrases. As soon as this most important fact is accepted, then necessarily the premise must be accepted that some descriptions will be significantly better than others for the study of particular properties of a process.

We have hinged our description of physical processes upon the <u>invariance concept</u>. By this we mean that we have consistently introduced state variables and written our equations in such a way as to stress the idea that any individual process is to be considered as a member of a family of related processes. The advantage to be gained from this point of view resides in the common observation that the properties of a particular member of a set can often be easily understood in terms of the properties of contiguous elements, although often quite puzzling to comprehend in isolation. This principle of continuity, one of the most powerful and versatile tools in the mathematicians hope chest, is basic also in the biological world.

The usual equations of mathematical physics arise from the application of imbedding techniques, by means of the introduction of fluxes at arbitrary points, by means of the introduction of time, and so on. By introducing other parameters of significance and applying invariance principles in a different fashion, we have obtained new equations which possess certain computational and analytic advantages over the classical formulations. We have indicated how one can pass back and forth from one type of equation to the other.

One of the major difficulties of the classical approach lies in the fact that it leads to boundary value problems which in turn lead to Fredholm integral equations. Ultimately for the solution of these problems in numerical terms we are forced to the solution of large systems of linear equations. This is a most subtle and difficult problem and one for which modern digital computers are not well suited.

The new approach presented here leads to the solution of initial value problems, not necessarily in time but in other meaningful physical parameters, and computationally to the iteration of nonlinear transformations. This latter is a task well designed for the digital computer. Finally, we note that our formulation very often corresponds to the way the data is obtained experimentally.

Let us note in passing that there are available other techniques for converting boundary value problems involving Fredholm type integral equations to initial value problems relying upon Volterra type integral equations. Generalizing

results of Holmgren and Levi, Muntz discussed how this could be done for the heat equation, while Milgram and Rosenbloom used a different device for treating generalized potential theory, involving the harmonic integrals of Hodge. Our methods are quite different from theirs, since ours always involve a variation of the domain, while theirs keep the domain fixed.

Secondly, let us point out that the Riccati equations which are characteristic of our approach can be obtained in a number of different ways in dealing with ordinary second order differential equations. The derivation we employ is quite different from that obtained by a simple change of a dependent variable, and different also from that resulting from dynamic programming. Our methods lead naturally to the generalized Riccati equations corresponding to partial differential operators.

The functions with which we deal, the reflection and transmission functions, appear to be basic functions of analysis. This is to be expected since they represent fundamental physical quantities. Using these functions we obtain a new approach to the problems of existence and uniqueness of solutions of the classical equations, and new representations for the solutions of these equations. What is most important is that these methods are independent of characteristic value and spectral theory. Results of this type will appear in the near future.

Although we have from time to time mentioned various computational advantages of our procedures, we have not included any calculations in this paper for several reasons. In the first place the paper has already assumed a certain unwieldy length. Far more important is the fact that numerical solution of significant problems introduce a number of nontrivial questions, regardless of the methods that is used. Any who have engaged in the computational solution of equations will sadly testify to this. Consequently, we feel that it is better to leave the calculations for a separate study, devoted merely to this aspect.

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